From Microscopic Interactions to Density Functionals

Von Mikroskopischen Wechselwirkungen hin zu Dichtefunktionalen
Zur Erlangung des Grades eines Doktors der Naturwissenschaften (Dr. rer. nat.)
genehmigte Dissertation von M.Sc. Sandra Karina Kemler, geb. in Offenbach am Main
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Fachbereich Physik
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Strongly Interacting Fermions

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Abstract

Density functional theory provides the basis for uncounted studies of ground-state properties of many-body systems. However, the connection between the energy density functional and the underlying microscopic interactions of a given theory is not fully understood. In this thesis we use renormalization-group techniques in combination with density functional theory to study many-body systems from microscopic interactions. We apply our formalism to different one-dimensional systems. We start with systems of identical fermions interacting via a short-range repulsive and long-range attractive interaction which serves as a simple one-dimensional toy model for nuclei. After that we study systems of spin-$1/2$ fermions, where we assume interactions only between fermions with different spins and consider both a non-local interaction as in the previous case and a contact interaction. In particular, the contact interaction plays a prominent role for ultracold *Fermi* gases. We calculate ground-state properties such as the energy, density, intrinsic density and density correlation functions and compare our results to values obtained from other approaches. Moreover, we show how energies of excited states and the absolute square of the ground-state wavefunction can be extracted from the density-density correlation function. The relation between our formalism and conventional density functional theory as well as many-body perturbation theory is discussed which may help to guide the development of ab initio functionals for quantitative studies of nuclei in the future.

Zusammenfassung

Die Dichtefunktionaltheorie stellt die Basis für unzählige Untersuchungen von Grundzustandseigenschaften von Vielteilchensystemen dar. Die Verbindung zwischen dem Energiedichtefunktional und der zugrundeliegenden Wechselwirkung einer gegebenen Theorie ist jedoch noch nicht vollständig verstanden. In dieser Arbeit nutzen wir Renormierungsgruppentechniken in Kombination mit Dichtefunktionaltheorie, um Vielteilchensysteme ausgehend von mikroskopischen Wechselwirkungen zu beschreiben. Wir wenden unseren Formalismus auf verschiedene eindimensionale Systeme an. Konkret untersuchen wir Systeme aus identischen Fermionen, die mittels einer kurzreichweitig abstoßenden und langreichweitig anziehenden Wechselwirkung miteinander wechselwirken. Dies stellt ein einfaches eindimensionales Kernmodell dar. Danach untersuchen wir Systeme mit Spin-$1/2$ Fermionen, wobei wir annehmen, dass nur Fermionen mit unterschiedlichem Spin miteinander wechselwirken. Für deren funktionale Form betrachten wir sowohl eine nichtlokale Wechselwirkung wie im Fall identischer Fermionen als auch eine Kontaktwechselwirkung. Wir berechnen Grundzustandseigenschaften wie zum Beispiel die Energie, Dichte, intrinsische Dichte und Dichte-Dichte-Korrelationsfunktionen dieser Systeme. Außerdem zeigen wir, wie Energien angeregter Zustände und das Betragsquadrat der Grundzustandswellenfunktion aus der Dichte-Dichte-Korrelationsfunktion abgeleitet werden können. Der Zusammenhang zwischen unserem Formalismus und konventioneller Dichtefunktionaltheorie ebenso wie der mit Vielteilchenstörungstheorie wird diskutiert. Dies kann helfen, zukünftig ab initio Funktionale für quantitative Untersuchungen von Kernen zu entwickeln.

Contents

1 Introduction

Density Functional Theory (DFT) has been developed by *Hohenberg* and *Kohn* in 1964 to study atoms with large numbers of electrons [1, 2]. Since then density functional theory has been successfully used to study a large variety of quantum systems with many degrees of freedom, ranging from electronic systems [3] and ultracold quantum gases [4] to (heavy) nuclei.

For heavy nuclei, DFT currently remains the only feasible approach for a calculation of ground-state properties [5]. Nuclei consist of nucleons interacting with one another. A microscopic treatment of large nuclei using many-body wavefunctions is difficult since the number of possible configurations rapidly increases with increasing particle numbers in the nucleus. The advantage of density functional theory is the description of the nuclear properties via the density of the protons and neutrons which scales more favorably to heavy nuclei.

The application of density functional theory to the nuclear many-body problem has been very successful and improved the understanding of nuclear properties, see Refs. [6, 7, 8, 9] and also Ref. [10] for a review. However, many density functional methods are based on fitting the parameters of a given ansatz for the density functional to experimental data and then applying the obtained results to other nuclei [11, 12]. The connection to ab initio approaches to nuclear structure and ultimately to QCD is not yet clear and needs further investigation. Therefore, a microscopic approach to density functional theory would be worthwhile. In recent years many efforts have been undertaken to construct energy density functionals from microscopic nucleon forces, e. g., in optimized density matrix expansions [13, 14]. This approach can also be used to obtain energy density functionals from chiral interactions [15, 16].

To develop a better understanding of the connection between energy density functionals and microscopic interactions, a renormalization-group (RG) inspired approach to DFT appears to be useful as it provides the possibility to calculate ground-state properties directly from the underlying microscopic interactions. The *Hohenberg-Kohn* energy density functional can be identified with the so-called two-particle-point-irreducible (2PPI) effective action which can be obtained from the path integral via a Legendre transformation with respect to sources coupled to the densities, see, e.g., Refs. [17, 18, 19] for reviews. The connection between the energy functional and the path integral can then be used to combine DFT with existing RG approaches. In this thesis, we employ a Renormalization Group approach to Density Functional Theory (DFT-RG approach) put forward in Refs. [20, 21] and developed further in Refs. [19, 22, 23]. For a general discussion of the properties of nPPI effective actions, we refer the reader to Ref. [24]. A discussion of the relation of our DFT-RG (2PPI-RG) approach to 2PI-RG equations can be found in Refs. [25, 26]. The basic idea underlying our approach is to start from a non-interacting system, which defines the initial point of the RG flow, and then to turn on the interaction gradually. This allows to study the "transition" from the energy density functional of the non-interacting system to the one of the fully interacting system under consideration, such as nuclei or trapped ultracold *Fermi* gases. Since this RG approach relies on an expansion of the density functional about the ground state, the latter is followed continously while the interaction is turned on in the flow.

Besides giving important conceptional discussions of this DFT-RG framework we apply it to fermionic systems in one dimension. Such systems are not only interesting from a theoretical point of view. In recent years experiments with ultracold fermionic atoms in highly anisotropic harmonic traps could be realized which allow the investigation of quasi one-dimensional systems [27, 28, 29, 30]. First, we study identical fermions interacting via a short-range repulsive and long-range attractive two-body interaction that mimics to some extent nucleon-nucleon interactions in one dimension. This model has been introduced in the context of *Monte-Carlo* simulations [31] and has already been used to benchmark other approaches, see, e. g., Ref. [32].

Moreover, we study systems of spin-$1/2$ fermions, where the interaction is assumed only between fermions with different spins. In dilute ultracold *Fermi* gases of, e. g., ^{6}Li, where the kinetic energy is low, the important process is s-wave scattering. Therefore it is reasonable to assume a contact interaction and also that there is no interaction between fermions with identical spins [33]. In ultracold *Fermi* gases it is also possible to tune the scattering length via *Feshbach* resonances, which allows to study the transition from weakly to strongly coupled systems in a controlled way [34]. In this limit, ultracold *Fermi* gases are good systems to model properties of strongly interacting many-body systems such as nuclei.

In this thesis we, cosider a DFT-RG approach that has been put forward in Refs. [20, 21] and developed further in Refs. [19, 22, 23]. We start with an introduction of conventional density functional theory in Chap. 2 based on the *Hohenberg-Kohn* theorem. We will give an overview over the *Kohn-Sham* equations, the local density approximation and the gradient expansion. Additionally, we will discuss the approach to density functional theory via the path integral.

In Chap. 3, the DFT-RG approach is introduced. We will discuss how a flow equation for the density functional can be calculated from microscopic interactions and detail how the ground-state properties of the interacting system can be computed. Moreover, we discuss that the computation of the absolute square of the ground-state wavefunction as well as the spectral function, which gives us access to the energies of excited states, is possible. We will also show how our approach is related to perturbation theory, the *Hartree* approximation and conventional DFT.

As a first study we then apply our DFT-RG framework to a simple zero-dimensional toy model in Chap. 4 to obtain an insight into the details of our DFT-RG approach. We then aim at a study of fermions in a one-dimensional periodic box which turns out to be convenient from a practical point of view. In Chap. 5, we introduce the setup of the box, give the initial conditions of the non-interacting system and discuss the specific flow equations in the box. In Chap. 6, we consider identical fermions interacting via a short-range repulsive and long-range attractive two-body interaction originally introduced to benchmark *Monte-Carlo* (MC) studies. Finally, in Chap. 7, we discuss systems of spin-$1/2$ fermions interacting via the same non-local interaction and also via a contact interaction. For both types of systems we discuss our results and compare them to results obtained from other approaches. Our conclusions and an outlook can be found in Chap. 8.

2 Density Functional Theory

Any discussion of Density Functional Theory (DFT) has to start with *Hohenberg* and *Kohn*. They showed in 1964 that there is a one-to-one correspondence between the wavefunction and the density of a system [1]. This allows an efficient description of many-body problems. This description owes its flexibility and versatility to the generality of the underlying concepts as the central object of DFT is the density.

Shortly after the introduction of *Schrödinger's* wave mechanics in 1926 the first approaches have been introduced to describe the energy of a system only in terms of the density of the system. The *Thomas-Fermi* theory is a simple prototype of a DFT [35, 36]. The advantage of describing a system in terms of the density rather than the wavefunction is obvious as the density just depends on d coordinates and not on dN coordinates, where d is the dimension and N the particle number.

The approach to describe a system just in terms of the density has not really been acknowledged until *Hohenberg* and *Kohn* could put it on solid ground by proving their theorem. *Walter Kohn* received the *Nobel* prize in 1998 "for his development of the density-functional theory". For more details on the history of DFT we refer the reader for example to *Walter Kohn's* Nobel Lecture [37].

2.1 Variational Principles

Variational principles are often used in quantum mechanics. They are especially useful if perturbative approaches are not applicable, like in strongly interacting systems such as nuclei or atoms in a trap near a *Feshbach* resonance. Density functional related methods like the *Kohn-Sham* method or the renormalization group approach, which we want to introduce here, can be related to variational principles.

The *Rayleigh-Ritz* method [38] is based on the two following theorems:

Theorem 1: *Let $\hat{H}$ be the Hamiltonian of a physical system, $\hat{H} = \hat{H}^*$ and let $\hat{H}$ be time independent. The spectrum of $\hat{H}$ is bound from below. Then the functional*

$$E[\Psi] = \frac{\left\langle \Psi \left| \hat{H} \right| \Psi \right\rangle}{\langle \Psi | \Psi \rangle} \tag{2.1}$$

is minimal if and only if $|\Psi\rangle$ is the ground-state wavefunction. For every other wavefunction $|\Psi\rangle$ the energy $E[\Psi]$ is greater than the ground-state energy E_{gs}:

$$E_{gs} \leq E[\Psi]\,. \tag{2.2}$$

Theorem 2: *Let $E[\Psi]$ be defined as in Eq.* (2.1)*. $E[\Psi]$ is stationary if $|\Psi\rangle$ is an eigenvector of $\hat{H}$. Each eigenvector of $\hat{H}$ is a stationary point of $E[\Psi]$.*

For the proofs of these two theorems we refer the reader to Ref. [39]. To obtain an approximation for the ground-state energy one starts with an ansatz for the wavefunction $|\Psi\rangle = \sum_{i=1}^{N} c_i |\Psi_i\rangle$, which is a linear combination of a finite set of basis functions $\{|\Psi_i\rangle\}$ and unknown parameters c_i. By minimizing the energy functional $E[\Psi]$, one then obtains an upper bound for the ground-state energy.

From these two theorems the so-called *Hellmann-Feynman* theorem is obtained, see, e. g., Ref. [40, 41]. We will come back to this theorem when we discuss the relation of our formalism to variational principles and conventional DFT in Sec. 3.6.

Hellmann-Feynman Theorem: *Let $\hat{H}$ be a Hamiltonian depending on a real parameter $\lambda \in \mathbb{R}$, $\hat{H} \equiv \hat{H}(\lambda)$ and $|\Psi(\lambda)\rangle$ a normalized eigenvector of $\hat{H} \equiv \hat{H}(\lambda)$. The spectrum of $\hat{H}$ is bound from below. The theorem then states:*

$$\frac{\mathrm{d}E(\lambda)}{\mathrm{d}\lambda} = \frac{\mathrm{d}}{\mathrm{d}\lambda}\left\langle \Psi(\lambda)\left|\hat{H}(\lambda)\right|\Psi(\lambda)\right\rangle = \left\langle \Psi(\lambda)\left|\frac{\partial \hat{H}(\lambda)}{\partial \lambda}\right|\Psi(\lambda)\right\rangle . \tag{2.3}$$

A proof of the *Hellmann-Feynman* theorem can be found in Ref. [42].

2.2 Hohenberg-Kohn Theorem

Hohenberg and *Kohn* could show that there is a one-to-one correspondence between the ground-state density and the ground-state wavefunction of a system. In 1964 they formulated their theorem for local, spin-independent, external potentials that lead to non-degenerate ground states [1]. The following discussion of the *Hohenberg-Kohn* theorem follows Ref. [3].

Let us consider a fermionic many-body system that can be described by a non-relativistic and time-independent Hamiltonian of the form

$$\hat{H} = \hat{T} + \hat{V}_{\mathrm{ext}} + \hat{U} , \tag{2.4}$$

where the kinetic energy operator $\hat{T}$ is given by

$$\hat{T} = -\frac{1}{2m}\sum_{i=1}^{N} \vec{\nabla}_i^2 \tag{2.5}$$

and $\hat{U}$ is a given interaction between the fermions,

$$\hat{U} = \sum_{\substack{i,j=1 \\ i<j}}^{N} U(\vec{x}_i, \vec{x}_j) = \frac{1}{2}\sum_{\substack{i,j=1 \\ i\neq j}}^{N} U(\vec{x}_i, \vec{x}_j) . \tag{2.6}$$

The potential $\hat{V}_{\mathrm{ext}}$ describes an external potential:

$$\hat{V}_{\mathrm{ext}} = \sum_{i=1}^{N} V(\vec{x}_i) . \tag{2.7}$$

Here, we assume that the external potential is local and spin-independent and the corresponding ground state is not degenerate. Moreover, $\rho_{\mathrm{gs}}(\vec{x})$ is the ground-state density corresponding to this N-particle ground state.

The many-body eigenstates $|\Psi\rangle$ corresponding to the Hamiltonian (2.4) can be calculated with the stationary *Schrödinger* equation:

$$\hat{H}\,|\Psi\rangle = E\,|\Psi\rangle \ . \tag{2.8}$$

For the derivation of the *Hohenberg-Kohn* theorem we consider all Hamiltonians of the form (2.4) with non-degenerate ground states and assume that the interaction $U(\vec{x}, \vec{y})$ is kept fixed.

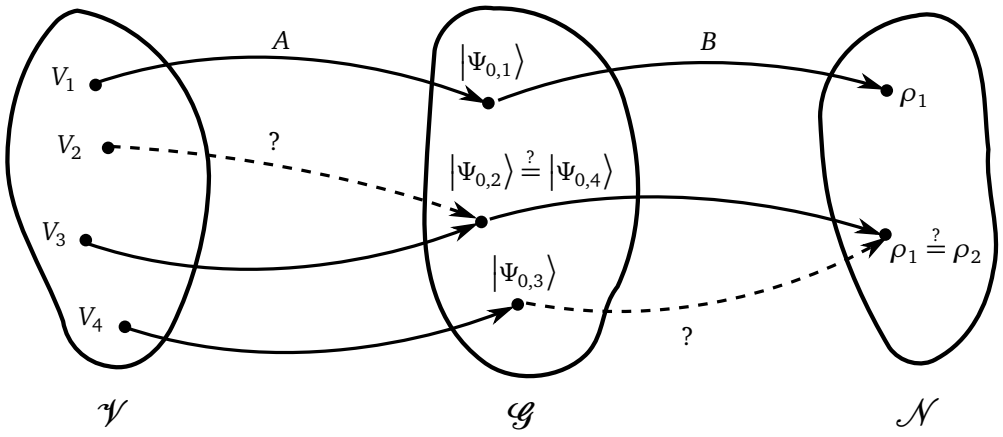

Figure 2.1.: Schematic representation of the correspondence between the external potential $V(x)$, the associated ground states $|\Psi_0\rangle$ and the ground-state densities $\rho_{\mathrm{gs}}(\vec{x})$.

We define the set $\mathscr{V}$ of all external potentials that lead to non-degenerate ground states

$$\mathscr{V} := \left\{ V \;\middle|\; V \text{ is local, corresponding ground state } |\Psi_0\rangle \text{ is not degenerate, } V' \neq V + \text{const.} \right\} \tag{2.9}$$

and the set $\mathscr{G}$ of all resulting ground states

$$\begin{aligned} \mathscr{G} := \Big\{ |\Psi_0\rangle \;\Big|\; & |\Psi_0\rangle \text{ is a ground state corresponding to one element of } \mathscr{V}, \\ & |\Psi_0'\rangle \neq \mathrm{e}^{\mathrm{i}\phi} |\Psi_0\rangle, \text{ with global phase } \phi \Big\}. \end{aligned} \tag{2.10}$$

We define a map $A : \mathscr{V} \to \mathscr{G}$ which is surjective by construction and one can show that it is also injective.

In the next step, we define the set $\mathscr{N}$ of all ground-state densities obtained from an element of $\mathscr{G}$:

$$\mathscr{N} := \left\{ \rho_{\mathrm{gs}} \;\middle|\; \rho_{\mathrm{gs}} = \langle \Psi_0 | \hat{\rho} | \Psi_0 \rangle, \; |\Psi_0\rangle \in \mathscr{G} \right\} \tag{2.11}$$

and a map $B : \mathscr{G} \to \mathscr{N}$. This map is again surjective by construction and can be shown to also be injective.

The two maps are illustrated in Fig. 2.1. Map A as well as map B are bijective and therefore invertible. By composition of these two maps we obtain a map $C : \mathscr{V} \to \mathscr{N}$ which is therefore also invertible. For this map *Hohenberg* and *Kohn* formulated their theorem:

Hohenberg-Kohn Theorem: *For an interacting system of N particles defined by a Hamiltonian of the form* (2.4) *the potential* $V(\vec{x})$ *is uniquely defined, this means up to an additive constant, by the ground-state density* $\rho_{\mathrm{gs}}(\vec{x})$.

A proof of the *Hohenberg-Kohn* theorem can be found in Ref. [3]. This theorem is the foundation of Density Functional Theory. Apart from the theorem itself we can deduce some fundamental statements from the considerations above. The external potential $V(\vec{x})$, the ground-state wavefunction $|\Psi_0\rangle$ and the ground-state density $\rho_{\mathrm{gs}}(\vec{x})$ determine each other uniquely. As a consequence of the invertibility of map B, the wavefunction can be written as a functional of the density $|\Psi[\rho]\rangle$ and the ground-state wavefunction is formally obtained by evaluating this wavefunctional at the ground-state density:

$$|\Psi_0\rangle = \left|\Psi[\rho_{\mathrm{gs}}]\right\rangle. \tag{2.12}$$

Note that an explicit knowledge of the external potential $V(\vec{x})$ is not needed here and that the functional form of $|\Psi[\rho]\rangle$ is the same for all systems with the same interaction potential $U(\vec{x}, \vec{y})$. The ground-state wavefunction of the N-particle system under consideration is therefore fully determined by the ground-state density even though

the functional form of $|\Psi[\rho]\rangle$ is not clear or easy to find. Moreover, there exists an unique functional of the exact ground-state density for every observable O:

$$O[\rho] := \langle \Psi[\rho] | \hat{O} | \Psi[\rho] \rangle \, . \tag{2.13}$$

This holds in particular for the ground-state energy and there exists an energy functional $E_{\mathrm{HK}}[\rho]$

$$E_{\mathrm{HK}}[\rho] := \langle \Psi[\rho] | \hat{H} | \Psi[\rho] \rangle = F_{\mathrm{HK}}[\rho] + \int \mathrm{d}^d x \, \rho(\vec{x}) V(\vec{x}) , \tag{2.14}$$

$$F_{\mathrm{HK}}[\rho] := \langle \Psi[\rho] | \hat{T} + \hat{U} | \Psi[\rho] \rangle \, . \tag{2.15}$$

With the *Rayleigh-Ritz* variational principle and the unique relation between ρ_{gs} and $|\Psi_0\rangle$ it follows that the ground-state density ρ_{gs} can be obtaind by minimizing $E_{\mathrm{HK}}[\rho]$ with respect to the density:

$$E_{\mathrm{gs}} = \min_{\rho \in \mathcal{N}} E_{\mathrm{HK}}[\rho] \, . \tag{2.16}$$

This defines the *Hohenberg-Kohn* variational principle. The energy functional $E_{\mathrm{HK}}[\rho]$ is restricted to the domain of densities that can be obtained from the solution of the *Schrödinger* equation, i. e. $\rho \in \mathcal{N}$.

The energy-density functional E_{HK} in the limit of vanishing external potential V is equal to the so-called *Hohenberg-Kohn* functional F_{HK}. For a given interaction potential U the functional F_{HK} is universal as one can see in Eq. (2.15). Moreover, one may also use the definition

$$F_{\mathrm{HK}}[\rho] = E_{\mathrm{HK}}[\rho] - \int \mathrm{d}^d x \, \rho(\vec{x}) V(\vec{x}) \, . \tag{2.17}$$

These considerations can be extended to degenerate ground states. We will not discuss this extension here but refer the reader to e. g., Ref. [3].

To use the variational principle in practice one would rather use the formulation

$$\left. \frac{\delta E_{\mathrm{HK}}[\rho]}{\delta \rho(\vec{x})} \right|_{\rho(\vec{x}) = \rho_{\mathrm{gs}}(\vec{x})} = 0 \tag{2.18}$$

instead of Eq. (2.16). The transition from the latter to Eq. (2.18) is not completely legitimate from a mathematical point of view. The definition of $E_{\mathrm{HK}}[\rho]$ requires $\rho(\vec{x})$ to be an element of $\mathcal{N}$ but the existence of the functional derivative $\delta E_{\mathrm{HK}}[\rho]/\delta\rho(\vec{x})$ requires the definition on a sufficiently dense set of densities. This rises the question if any well-behaved positive function $\rho(\vec{x})$ integrating to a positive integer N is a possible ground-state density that corresponds to some $V(\vec{x})$. Such a density is called V-representable. It is possible to find explicit counterexamples for densities that are not V-representable, see, e. g., Ref. [43]. To solve the V-representability problem one can find a suitable extension of $E_{\mathrm{HK}}[\rho]$ to ensure that the functional derivative $\delta E_{\mathrm{HK}}[\rho]/\delta\rho(\vec{x})$ exists [43, 44, 45]. For a more detailed discussion of the issue of V-representability and a general introduction to DFT we refer the reader to Refs. [3, 46, 47].

The *Hohenberg-Kohn* theorem is the starting point of an efficient description of many-body problems. It allows to describe the system under consideration with the ground-state density depending on d coordinates and not with the wavefunction which depends on dN coordinates. Unfortunately, the theorem does not provide a recipe on how to calculate the functional.

2.3 Kohn-Sham Equations

Kohn and *Sham* studied inhomogeneous systems of interacting electrons [2]. They discussed DFT by mapping an interacting many-body problem onto a suitable non-interacting system. This is realized by introducing a suitable background potential and leads to the so-called *Kohn-Sham* equations that we want to introduce in this section. We will neglect spin degrees of freedom here for simplicity but one can straightforwardly extend the method to systems with spin. Also the formalism can be extended to systems with degenerate ground states, see, e. g., Ref. [3].

We start by looking at a non-interacting system of N particles defined by the Hamiltonian

$$\hat{H}_\mathrm{s} = \hat{T} + \hat{V}_\mathrm{s}\,, \tag{2.19}$$

where the index "s" stands for "single particle". We assume that the ground state of $\hat{H}$ is non-degenerate. From the *Hohenberg-Kohn* theorem we can deduce that the energy-density functional $E_\mathrm{s}[\rho]$ in this case has the form:

$$E_\mathrm{s}[\rho] = T_\mathrm{s}[\rho] + \int \mathrm{d}^d x\, \rho(\vec{x})\, V(\vec{x})\,, \tag{2.20}$$

$$F_\mathrm{HK,s}[\rho] := T_\mathrm{s}[\rho] = \langle \Psi[\rho] |\, \hat{T}\, | \Psi[\rho] \rangle\ . \tag{2.21}$$

By a variation of $E_\mathrm{s}[\rho]$ with respect to the density $\rho(\vec{x})$, the ground-state density $\rho_\mathrm{s}(\vec{x})$ can be determined:

$$E_\mathrm{gs} = \min_\rho E_s[\rho] \quad \Rightarrow\ \rho_\mathrm{s}(\vec{x})\,. \tag{2.22}$$

The *Schrödinger* equation for N non-interacting fermions reads:

$$\left(-\frac{1}{2m}\vec{\nabla}^2 + V_\mathrm{s}(\vec{x})\right)\phi_i(\vec{x}) = \epsilon_i\, \phi_i(\vec{x}) \qquad \text{with } i = 1, \ldots, N\,, \tag{2.23}$$

where $\epsilon_1 \leq \epsilon_2 \leq \cdots \leq \epsilon_N$ and the set $\{\epsilon_i\}$ contains the eigenvalues of the N lowest single-particle orbitals $\phi_i(\vec{x})$ of the *Schrödinger* equation (2.23). Per construction the ground-state density $\rho_\mathrm{s}(\vec{x})$ can be expressed with the single particle orbitals:

$$\rho_\mathrm{s}(\vec{x}) = \sum_{i=1}^{N} |\phi_i(\vec{x})|^2\ . \tag{2.24}$$

The key aspect of the *Kohn-Sham* scheme is to assume that there exists a local single-particle potential V_s for every interacting system such that:

$$\rho_\mathrm{I}(\vec{x}) \equiv \rho_\mathrm{s}(\vec{x}) = \sum_{i=1}^{N} |\phi_i(\vec{x})|^2\,, \tag{2.25}$$

where $\rho_\mathrm{I}(\vec{x})$ is the corresponding density of the interacting N-particle system defined by the Hamiltonian (2.4). This means it is assumed that the interacting V-representable densities are also non-interacting V-representable.

The energy functional for the interacting system is defined by (2.14):

$$E_V[\rho] = F_\mathrm{HK}[\rho] + \int \mathrm{d}^d x\ \rho(\vec{x})\, V(\vec{x})\,. \tag{2.26}$$

As a consequence of the *Hohenberg-Kohn* theorem the single-particle orbitals are unique functionals of the density $\rho_\mathrm{s}(\vec{x})$ and therefore of $\rho_\mathrm{I}(\vec{x})$. In addition, $T_\mathrm{s}[\rho]$ is a functional of $\rho_\mathrm{I}(\vec{x})$. We will now rewrite the energy functional $E_V[\rho]$ (2.26):

$$E_V[\rho] = T_\mathrm{s}[\rho] + E_\mathrm{ext}[\rho] + E_\mathrm{Hartree}[\rho] + E_\mathrm{xc}[\rho]\,, \tag{2.27}$$

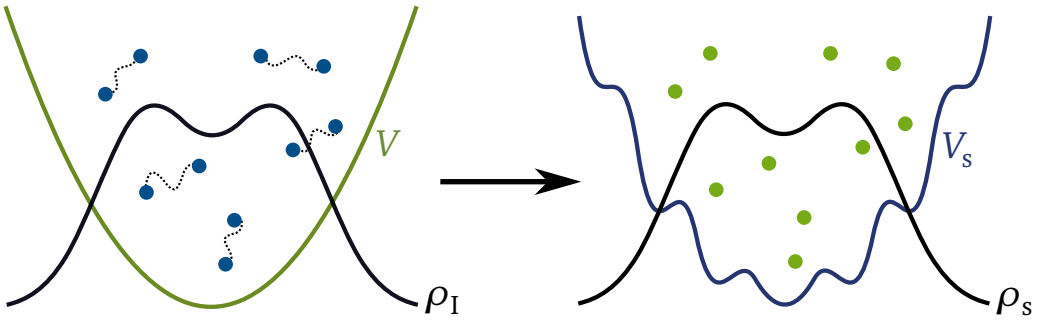

Figure 2.2.: Schematic illustration of the *Kohn-Sham* scheme. Left panel: The interacting system with potential V and ground-state density ρ_I. Right panel: The *Kohn-Sham* system with the effective potential V_s and ground-state density ρ_s. The density is identical in each case, $\rho_I = \rho_s$.

where $T_s[\rho]$ is the single-particle kinetic energy, the second term is the external energy

$$E_{ext}[\rho] = \int d^d x \, \rho(\vec{x}) V(\vec{x}), \tag{2.28}$$

which describes the coupling of the particles to the external potential $V(\vec{x})$. The third term is the so called *Hartree* energy

$$E_{Hartree}[\rho] = \frac{1}{2} \int d^d x \int d^d x' \, \rho(\vec{x}) U(\vec{x}, \vec{x}') \rho(\vec{x}') \tag{2.29}$$

and the last term $E_{xc}[\rho]$ is the exchange-correlation functional,

$$E_{xc}[\rho] = F_{HK}[\rho] - \frac{1}{2} \int d^d x \int d^d x' \, \rho(\vec{x}) U(\vec{x}, \vec{x}') \rho(\vec{x}') - T_s[\rho]. \tag{2.30}$$

The index “x” in “xc” stands for “exchange” or the consideration of the *Pauli* principle and the index “c” stands for “correlation”. $E_{xc}[\rho]$ contains all corrections to the *Hartree* term and as $F_{HK}[\rho]$ contains a kinetic term, the exchange correlation functional contains a kinetic part as well as an interaction part.

By using the *Hohenberg-Kohn* variational principle it is possible to obtain an expression for $V_s(\vec{x})$:

$$V_s(\vec{x}) = V(\vec{x}) + V_{Hartree}(\vec{x}) + V_{xc}[\rho](\vec{x}), \tag{2.31}$$

where the second term is the so called *Hartree* potential:

$$V_{Hartree}(\vec{x}) = \int d^d x' \, U(\vec{x}, \vec{x}') \rho_I(\vec{x}') \tag{2.32}$$

and the exchange-correlation potential is defined as

$$V_{xc}[\rho](\vec{x}) = \frac{\delta E_{xc}}{\delta \rho(\vec{x})}. \tag{2.33}$$

The exact single-particle potential $V_s(\vec{x})$ represents an effective potential. For non-interacting particles it yields the exact same density as for the interacting system. So it is possible to map the interacting N-body system onto a

non-interacting N-body system. In Fig. 2.2 this mapping is illustrated. The set of Eqs. (2.23), (2.31) and (2.25) are called the *Kohn-Sham* equations:

$$\left(-\frac{1}{2m}\vec{\nabla}^2 + V_\mathrm{s}(\vec{x})\right)\phi_i(\vec{x}) = \epsilon_i\,\phi_i(\vec{x})$$
$$V_\mathrm{s}(\vec{x}) = V(\vec{x}) + \int \mathrm{d}^d x'\; U(\vec{x},\vec{x}')\,\rho_\mathrm{I}(\vec{x}') + V_\mathrm{xc}[\rho_\mathrm{I}](\vec{x})$$
$$\rho_\mathrm{I}(\vec{x}) = \rho_\mathrm{s}(\vec{x}) = \sum_{i=1}^{N} |\phi_i(\vec{x})|^2\,,$$

where $\epsilon_1 \leq \epsilon_2 \leq \cdots \leq \epsilon_N$. The *Kohn-Sham* equations together with the statement that it is possible to depict an interacting N-body problem on a non-interacting N-body problem is also called *Kohn-Sham* theorem.

The *Kohn-Sham* equations are a non-linear set of equations. The *Kohn-Sham* orbitals $\{\phi_i(\vec{x})\}$ depend on the potential $V_\mathrm{s}(\vec{x})$ which depends on the density, which depends on the orbitals. This means that we have to solve the *Kohn-Sham* equations self-consistently. The initial density can be chosen freely but one should take into account the physical conditions, like symmetry, to accomplish a faster convergence. From the density it is then possible to deduce all other physical observables due to the *Hohenberg-Kohn* theorem. The ground-state energy for example can be calculated as follows:

$$\begin{aligned} E_\mathrm{gs} \equiv E_V[\rho_\mathrm{I}] &= T_\mathrm{s}[\rho_\mathrm{I}] + \int \mathrm{d}^d x\;\rho_\mathrm{I}(\vec{x})\,V(\vec{x}) + \frac{1}{2}\int \mathrm{d}^d x \int \mathrm{d}^d x'\;\rho_\mathrm{I}(\vec{x})\,U(\vec{x},\vec{x}')\,\rho_\mathrm{I}(\vec{x}') + E_\mathrm{xc}[\rho_\mathrm{I}] \\ &= T_\mathrm{s}[\rho_\mathrm{I}] + \int \mathrm{d}^d x\;\rho_\mathrm{I}(\vec{x})\,V_\mathrm{s}(\vec{x}) - \int \mathrm{d}^d x\;\rho_\mathrm{I}(\vec{x})\,V_\mathrm{xc}(\vec{x}) - \frac{1}{2}\int \mathrm{d}^d x \int \mathrm{d}^d x'\;\rho_\mathrm{I}(\vec{x})\,U(\vec{x},\vec{x}')\,\rho_\mathrm{I}(\vec{x}') + E_\mathrm{xc}[\rho_\mathrm{I}] \\ &= \sum_{i=1}^{N}\epsilon_i - \int \mathrm{d}^d x\;\rho_\mathrm{I}(\vec{x})\,V_\mathrm{xc}(\vec{x}) - \frac{1}{2}\int \mathrm{d}^d x \int \mathrm{d}^d x'\;\rho_\mathrm{I}(\vec{x})\,U(\vec{x},\vec{x}')\,\rho_\mathrm{I}(\vec{x}') + E_\mathrm{xc}[\rho_\mathrm{I}]\,. \end{aligned} \tag{2.34}$$

Neither the *Kohn-Sham* single-particle orbitals nor the energies ϵ_i have a physical meaning, besides the calculation of the density from the orbitals (2.25). As we see in Eq. (2.34), the ground-state energy is not just the sum over all ϵ_i. If one studies spectra of atoms within this DFT formalism it is possible to show that the energy of the highest occupied orbital ϵ_N is the negative ionzation energy [48]. Also the N-particle wavefunction which comes out of the *Kohn-Sham* equations is not identical with the exact ground-state wavefunction. Only the following relation holds:

$$\rho_\mathrm{I}(\vec{x}) = \langle\Psi_\mathrm{I}\,|\hat{\rho}\,|\,\Psi_\mathrm{I}\rangle = \langle\Psi_\mathrm{s}\,|\hat{\rho}\,|\,\Psi_\mathrm{s}\rangle = \rho_\mathrm{s}(\vec{x})\,, \tag{2.35}$$

where $|\Psi_\mathrm{I}\rangle$ is the N-particle state vector obtained by the *Kohn-Sham* equations and $|\Psi_\mathrm{s}\rangle$ is the exact ground-state vector.

The *Hartree* term in the *Kohn-Sham* potential V_s corresponds to a mean-field approximation. If one neglects V_xc one obtains the *Hartree* approximation. The DFT itself is not a mean-field approximation of the N-particle problem but a reorganisation of the many-body problem with the help of a mean-field reference state. If we solve the *Kohn-Sham* equations exactly, we have taken into account all quantum effects. Loosely speaking, the *Kohn-Sham* equations are therefore the formal exactification of the *Hartree* theory.

During the iteration process we need to determine V_s. This potential depends on the unknown quantity V_xc, which in general we have to calculate approximately. With this we have shifted the task to solve the *Schrödinger* equation, which for large particle numbers N is impossible, to the computation of the potential V_xc. Thus, we are left with the question whether it is possible to find a systematic approximation of V_xc.

2.4 Local Density Approximation and Gradient Expansion

There are in principle two possible ways to determine a ground state of a system within the DFT framework: The first is to find an approximation for E_{xc} and solve the *Kohn-Sham* equations self-consistently and the second is to find an approximation for the *Hohenberg-Kohn* functional F_{HK} and directly apply the *Hohenberg-Kohn* variational principle.

In general, it is difficult to find a systematic and stable approximation for E_{xc} or F_{HK}. The Local Density Approximation (LDA) is a simple approximation that uses the density dependence of the ground-state energy of the corresponding homogeneous many-body problem. The constant density is then replaced by the inhomogeneous density $\rho_{\mathrm{gs}}(\vec{x})$. For the exchange-correlation functional E_{xc} this means

$$E_{\mathrm{xc}}^{\mathrm{LDA}}[\rho] = \int \mathrm{d}^d x \; \mathscr{E}_{\mathrm{xc}}^{\mathrm{LDA}}(\rho(\vec{x})), \tag{2.36}$$

$$\mathscr{E}_{\mathrm{xc}}^{\mathrm{LDA}}(\rho(\vec{x})) = \mathscr{E}_{\mathrm{xc}}^{\mathrm{hom}}(n_0)\Big|_{n_0\to\rho(\vec{x})}, \tag{2.37}$$

where $\mathscr{E}_{\mathrm{xc}}^{\mathrm{hom}}$ is the exchange-correlation energy per volume for the uniform *Fermi* gas with homogeneous density n_0. The ground-state energy density of the homogenous system can for example be derived through Monte-Carlo simulations.

It is possible to show that LDA represents the lowest order in a systematic gradient expansion of the exact energy-density functional [49]. A low-order approximation might only be justified in systems with weakly varying densities, such as ultracold Fermi gases with a large number of atoms in an isotropic trap [50]. In general, however, a gradient expansion may have bad convergence properties.

To motivate the statement that one can find a gradient expansion for the energy-density functional or related quantities we start from an expansion of a general functional $\mathscr{F}$ about the homogeneous ground-state density n_{gs}:

$$\mathscr{F}[\rho] = \mathscr{F}^{(0)}(n_{\mathrm{gs}}) + \frac{1}{2}\int \mathrm{d}^d x_1 \int \mathrm{d}^d x_2 \; \left(\rho(\vec{x}_1) - n_{\mathrm{gs}}\right) \; \mathscr{F}^{(2)}(n_{\mathrm{gs}}; \vec{x}_1, \vec{x}_2) \; \left(\rho(\vec{x}_2) - n_{\mathrm{gs}}\right) + \dots . \tag{2.38}$$

For example, $\mathscr{F}$ can be associated with E_{HK}, F_{HK} or E_{xc}. The expansion coefficients are given by:

$$\mathscr{F}^{(m)}(n_{\mathrm{gs}}; \vec{x}_1, \dots, \vec{x}_m) = \frac{\delta^m \mathscr{F}[\rho]}{\delta\,\rho(\vec{x}_1)\dots\delta\,\rho(\vec{x}_m)}\bigg|_{\rho=n_{\mathrm{gs}}}. \tag{2.39}$$

Assuming that the many-body system under consideration is invariant under $\vec{x}_i \to -\vec{x}_i$ and translations $\vec{x}_i \to \vec{x}_i + \vec{a}$ with $\vec{a}$ defining an arbitrary shift, the expansion (2.38) can be recast into a gradient expansion of the following form [51]:

$$\mathscr{F}[n] = \mathscr{F}^{\mathrm{LDA}}[\rho] + \int \mathrm{d}^d x \; \tilde{G}^{(2)}(\rho(\vec{x})) \left(\vec{\nabla}\,\rho(\vec{x})\right)^2 + \dots . \tag{2.40}$$

In contradistinction to the expansion (2.38) of the functional $\mathscr{F}$, the derivative expansion (2.40) does not depend on the ground-state density n_{gs} anymore, this means it is a global functional rather than a local approximation. The new quantities appearing in the derivative expansion can in principle be derived from the correlation functions $\mathscr{F}^{(m)}$. The first term on the right-hand side of Eq. (2.40) is associated with LDA which can also be obtained from $\mathscr{F}^{(m)}$ and its derivatives with respect to a homogeneous “trial” density. The correlation function $\tilde{G}^{(2)}$ is fully determined by the derivatives of the Fourier transform of $\mathscr{F}^{(2)}$ with respect to a homogeneous ”trial“ density. Note that we assume that the radius of convergence of the expansion (2.38) is infinite. This relation between the two expansions is a direct consequence of the fact that the correlation functions $\mathscr{F}^{(m)}$ obey the following relation:

$$\frac{\partial\,\mathscr{F}^{(m)}(\vec{x}_1, \dots, \vec{x}_m)}{\partial\, n_{\mathrm{gs}}} = \int \mathrm{d}^d x_{m+1} \; \mathscr{F}^{(m+1)}(\vec{x}_1, \dots, \vec{x}_{m+1}). \tag{2.41}$$

In principle, the gradient expansion contains derivative terms of arbitrarily high orders in Eq. (2.40). To compute the term of order $\mathcal{O}(\vec{\nabla}^4)$ for example one needs the correlation function $\mathscr{F}^{(4)}$ as input. It is difficult to estimate if such a gradient expansion is valid and if the radius of convergence is really infinite. The analysis in general requires the knowledge of the underlying correlation functions $\mathscr{F}^{(m)}$. Depending on the system under consideration, the gradient expansion may therefore be only of limited use.

We will come back to this translation between the gradient expansion and the expansion (2.38) about the ground state later when we relate our RG-approach to conventional DFT as explained in this chapter. For this purpose we provide the expansion for E_{HK} about the homogeneous ground-state density n_{gs} and the gradient expansion for E_{HK} in one dimension:

$$E_{\mathrm{HK}}[n] = E_{\mathrm{HK}}^{(0)} + \frac{1}{2}\int \mathrm{d}x_1 \int \mathrm{d}x_2 \, \big(n(x_1) - n_{\mathrm{gs}}\big)\, E_{\mathrm{HK}}^{(2)}(x_1, x_2)\, \big(n(x_2) - n_{\mathrm{gs}}\big) + \dots , \tag{2.42}$$

$$E_{\mathrm{HK}}[n] = g_{\mathrm{HK}}^{(0)}[n] + \int \mathrm{d}x \; g_{\mathrm{HK}}^{(2)}(n) \left(\frac{\partial n(x)}{\partial x}\right)^2 + \dots . \tag{2.43}$$

2.5 Density Functional Theory and the Path Integral Formalism

In this work we choose a path integral approach to Density Functional Theory. In this section we want to show how the path integral representation for the effective action can be related to the density functional. For a detailed introduction of path integrals and especially the fermionic path integral, see, e. g., Ref. [52].

We start from the grand canonical partition function Z :

$$Z = \mathrm{Tr}\, \mathrm{e}^{-\beta(\hat{H} - \mu \hat{N})}, \tag{2.44}$$

where μ is the chemical potential and $\hat{N}$ is the particle number operator defined by:

$$\hat{N} = \int \mathrm{d}^d x \, \sum_\sigma \hat{\psi}_\sigma^\dagger(\vec{x}) \hat{\psi}_\sigma(\vec{x}), \tag{2.45}$$

where the σ-sum is over all possible spin states. We use the imaginary time formalism throughout this work, where $t \to -\mathrm{i}\tau$ and the extent of the imaginary-time axis can be identified with $\beta = 1/T$. The path integral representation of the partition function in the grand-canonical potential reads:

$$Z \sim \int\limits_{\psi_\sigma(\beta,\vec{x}) = -\psi_\sigma(0,\vec{x})} \mathscr{D}\psi_\sigma^\dagger \mathscr{D}\psi_\sigma \; \mathrm{e}^{-\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d x \left\{ \mathscr{L}[\psi^\dagger,\psi] - \mu \sum_\sigma \psi_\sigma^\dagger(\tau,\vec{x})\psi_\sigma(\tau,\vec{x}) \right\}}, \tag{2.46}$$

where we dropped an irrelevant normalization factor. $\mathscr{L}$ is the Lagrange density corresponding to the Hamiltonian (2.4):

$$\begin{aligned} \mathscr{L}[\psi^\dagger,\psi] = &\sum_\sigma \psi_\sigma^\dagger(\tau,\vec{x}) \left[\frac{\partial}{\partial\tau} - \frac{1}{2}\Delta + V(\vec{x})\right] \psi_\sigma(\tau,\vec{x}) \\ &+ \frac{1}{2}\sum_{\sigma\sigma'} \int \mathrm{d}^d x' \; \psi_\sigma^\dagger(\tau,\vec{x}) \psi_{\sigma'}^\dagger(\tau',\vec{x}') U(\vec{x},\vec{x}') \psi_{\sigma'}(\tau',\vec{x}') \psi_\sigma(\tau,\vec{x}) \end{aligned} \tag{2.47}$$

and the classical action S is defined by

$$S[\psi^\dagger,\psi] = \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d x \; \mathscr{L}[\psi^\dagger,\psi]. \tag{2.48}$$

Now we would like to make contact between the effective action approach to quantum field theory and density functional theory, see, e. g., Ref. [17, 18] for a more detailed introduction. To obtain the effective action we introduce external sources $\{J_\sigma\}$ into the path integral:

$$\begin{aligned} Z[\{J_\sigma\}] &\sim \int \mathscr{D}\psi_\sigma^\dagger \mathscr{D}\psi_\sigma \, \mathrm{e}^{-S[\psi^\dagger,\psi]+\sum_\sigma \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d x \; J_\sigma(\tau,\vec{x})(\psi_\sigma^\dagger(\tau,\vec{x})\psi_\sigma(\tau,\vec{x}))} \\ &\equiv \mathrm{e}^{W_V[\{J_\sigma\}]} . \end{aligned} \tag{2.49}$$

Note that we coupled a term bilinear in the fermion fields to the external sources $\{J_\sigma\}$. The chemical potential μ can be absorbed in the external sources as a constant shift. From Eq. (2.49), we obtain the generating functional of the connected density correlation functions

$$W_V[\{J_\sigma\}] = \ln Z[\{J_\sigma\}] . \tag{2.50}$$

We now introduce the classical fields $\rho_\sigma(\tau,\vec{x})$ that are defined as the derivative of the functional $W[\{J_\sigma\}]$ with respect to the sources $J_\sigma(\tau,\vec{x})$

$$\rho_\sigma(\tau,\vec{x}) := \frac{\delta W_V[\{J_\sigma\}]}{\delta J_\sigma(\tau,\vec{x})} . \tag{2.51}$$

Here, the classical fields ρ_σ are not only functions of τ and $\vec{x}$ but also functionals of the sources $\{J_\sigma\}$, i. e. $\rho_\sigma = \rho_\sigma[\{J_\sigma\}]$. These fields are directly connected to the particle densities, as we will discuss later.

Performing a Legendre transformation of W_V with respect to the sources J_σ we obtain the 2PPI[1] effective action:

$$\Gamma_V[\{\rho_\sigma\}] = \sup_{\{J_\sigma\}} \left\{ -W_V[\{J_\sigma\}] + \sum_\sigma \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d x \; J_\sigma(\tau,\vec{x})\rho_\sigma(\tau,\vec{x}) \right\} . \tag{2.52}$$

This 2PPI effective action $\Gamma_V[\{\rho_\sigma\}]$ contains the complete dynamics of the many-body system. Phenomenologically, this transformation to the 2PPI effective action may be viewed as a bosonization of the theory since we have traded in the fermion fields in the classical action S for the composite bosonic fields ρ_σ in the effective action Γ_V. For a more general discussion of density-functional theory in terms of Legendre transformations, see, e. g., Refs. [53, 54].

It is straightforward to see that the 2PPI effective action $\Gamma_V[\{\rho_\sigma\}]$ does not depend on the sources $\{J_\sigma\}$:

$$\frac{\delta \Gamma_V[\{\rho_\sigma\}]}{\delta J_\sigma} = 0 . \tag{2.53}$$

The quantum equation of motion of ρ_σ follows from

$$\frac{\delta \Gamma_V[\{\rho_\sigma\}]}{\delta \rho_\sigma(\tau,\vec{x})} = J_\sigma(\tau,\vec{x}) \tag{2.54}$$

in the limit $J_\sigma \to 0$, being the analogue of the *Hohenberg-Kohn* variational principle. The ground-state configuration $\{\rho_{\mathrm{gs},\sigma}\}$ is determined through the limit $J_\sigma \to 0$ of Eq. (2.54). Solving this equation for the fields $\rho_\sigma(\tau,\vec{x})$ in this limit we obtain the ground-state densities $\{\rho_{\mathrm{gs},\sigma}\}$.

With the results $\{\rho_{\mathrm{gs},\sigma}\}$ we can then obtain the ground-state energy E_{gs} of the system:

$$E_{\mathrm{gs}} = \lim_{\beta\to\infty} \frac{1}{\beta} \Gamma_V[\{\rho_{\mathrm{gs},\sigma}\}] = -\lim_{\beta\to\infty} \frac{1}{\beta} W_V[0] , \tag{2.55}$$

[1] "2PPI" stands for "two-particle point-irreducible" [21, 19]. A 2PPI diagram is a 1PI diagram that cannot be split into two by cutting two internal lines attached to the same vertex. Here, we obtain this type of effective action because in the path integral we coupled a local source term to a term bilinear in the fields.

which follows from Eq. (2.50) and the spectral representation of the partition function

$$Z \sim \sum_n \mathrm{e}^{-\beta E_n}\,, \tag{2.56}$$

where $E_{gs} \equiv E_0 < E_1 < E_2 < \ldots$ and the set $\{E_n\}$ denotes the energy spectrum associated with the many-body system under consideration. Again, we assume that the ground state is not degenerate.

The 2PPI effective action Γ_V can be related to the energy-density functional mentioned in context of the *Hohenberg-Kohn* DFT formalism, see Sec. 2.2. We can obtain the relation between the effective action Γ_V and the energy-density functional E_{HK} (2.14) from Eq. (2.55):

$$E_{\mathrm{HK}}[\{\rho_\sigma\}] = \lim_{\beta\to\infty} \frac{1}{\beta}\Gamma_V[\{\rho_\sigma\}]\,. \tag{2.57}$$

The universality of the *Hohenberg-Kohn* functional E_{HK} follows from the fact that the background potential can be absorbed in the sources J_σ by introducing a simple transformation $J_\sigma \to J_\sigma + V$, see, e. g., Ref. [21]. With this we find

$$\Gamma_V[\{\rho_\sigma\}] = \Gamma_{\mathrm{HK}}[\{\rho_\sigma\}] + \sum_\sigma \int_0^\beta \mathrm{d}\tau \int \mathrm{d}^d x\; V(\vec{x})\rho_\sigma(\tau,\vec{x})\,, \tag{2.58}$$

where $\Gamma_{\mathrm{HK}}[\{\rho_\sigma\}] = \Gamma_{V=0}[\{\rho_\sigma\}]$.

We conclude that the functional $\Gamma_{\mathrm{HK}}[\{\rho_\sigma\}]$ is only dependent on the interaction potential U and not on the background potential V and can therefore be associated with the universal *Hohenberg-Kohn* functional F_{HK} . We emphasize that the ground-state density ρ_σ depends in general on the time τ while the classical *Hohenberg-Kohn* functional is only dependent on time-independent densities, see, e. g., Refs. [55, 56, 20, 57]. In this sense, the path-integral construction of the energy-density functional Γ_{HK} leads to a generalization of the energy-density functional E_{HK} as defined by *Hohenberg* and *Kohn*.

3 Renormalization Group Approach to Density Functional Theory

In this chapter we will describe our Renormalization Group approach to Density Functional Theory (DFT-RG approach) that has been put forward in Refs. [20, 21] and developed further in Refs. [19, 22, 23]. We derive the flow equation for the energy density functional as well as the generating functional of the connected density correlation functions for a system of fermions in one dimension and give a general discussion of field-theoretical aspects of our DFT-RG approach. We would like to add that the generalization of this part of our work to higher dimensions is comparatively straightforward.

In particular, we derive the flow equations for the energy, the density and the density correlation functions and show how the absolute square of the wavefunction and the spectral function can be calculated from the density-density correlation function. We discuss the connection of our approach to many-body perturbation theory and the *Hartree* approximation. The DFT-RG approach is also related to conventional DFT as discussed in the last chapter.

The system under consideration has N_σ fermions with spin σ. The total number of fermions N is then obtained by $N = \sum_\sigma N_\sigma$, where we sum over all possible spin states. In Chap. 7, for example, we will assume that the fermions can either be spin-up fermions or spin-down fermions.

3.1 Flow Equation for the Energy Density Functional

Starting from the so-called classical action and the path integral, we derive a flow equation for the energy density functional describing the dynamics of a system of fermions interacting via a general two-body interaction. From this equation, flow equations for the density correlation functions can then be obtained. For convenience, we restrict the following discussion to the one-dimensional case but it can be extended to higher dimensions straightforwardly. The classical action S defining the many-body problem under consideration in this work is given by

$$\begin{aligned} S_\lambda[\psi^*,\psi] = &\sum_\sigma \int_\tau \int_x \psi^*_\sigma(\tau,x)\left(\partial_\tau - \frac{1}{2}\partial_x^2 + V(x)\right)\psi_\sigma(\tau,x) \\ &+ \frac{1}{2}\sum_{\sigma\sigma'}\int_\tau\int_x\int_{\tau'}\int_{x'} \psi^*_\sigma(\tau,x)\,\psi^*_{\sigma'}(\tau',x')\,U_{2\mathrm{b},\sigma\sigma'}(\tau,x,\tau',x')\,\mathscr{R}_\lambda(\tau,x,\tau',x')\,\psi_{\sigma'}(\tau',x')\psi_\sigma(\tau,x), \end{aligned} \tag{3.1}$$

where we have set $m = 1$ for the mass of the fermions and introduced the shorthands $\int_\tau = \int_{-\infty}^{\infty} \mathrm{d}\tau$, $\int_x = \int_{-\infty}^{\infty}\mathrm{d}x$, $\partial_\tau = \frac{\partial}{\partial\tau}$, and $\partial_x = \frac{\partial}{\partial x}$. The function $U_{2\mathrm{b},\sigma\sigma'}(\tau,x,\tau',x') = \delta(\tau-\tau')U_{\sigma\sigma'}(x-x')$ describes an instantaneous two-body (2b) interaction and $\mathscr{R}_\lambda$ is a (dimensionless) regulator function which obeys the following conditions:

$$\lim_{\lambda\to 0}\mathscr{R}_\lambda(\tau,x,\tau',x') = 0 \quad \text{and} \quad \lim_{\lambda\to 1}\mathscr{R}_\lambda(\tau,x,\tau',x') = 1\,. \tag{3.2}$$

Here, $\lambda \in [0,1]$ is a dimensionless control parameter. The first condition ensures that the two-body potential U is switched off for $\lambda = 0$ and we are left with a system of non-interacting fermions in a background potential V. For $\lambda = 1$, the second condition ensures that U is fully switched on and the action (3.1) describes fermions in the background potential V interacting via the two-body interaction U. Other than the two conditions in Eq. (3.2), the

function $\mathscr{R}_\lambda$ is at our disposal.[1] For convenience, however, we shall also assume that this function does not break the symmetries of the theory under consideration.

For studies in higher dimensions ($d > 1$), a suitable choice for $\mathscr{R}_\lambda$ may indeed be required to control ultraviolet divergences, e. g., in systems of fermions with an internal degree of freedom interacting via a contact interaction. In any case, we are free to choose $\mathscr{R}_\lambda$ such that the change in the parameter λ corresponds to a change of a momentum scale or, correspondingly, a length scale. For example, λ may effectively correspond to an upper bound for the range of the interaction associated with the two-body potential U. In this case, the regulator function $\mathscr{R}_\lambda$ is designed such that an increase of λ corresponds to an increase of this effective upper bound starting from zero at $\lambda = 0$ and approaching infinity for $\lambda \to 1$. Assuming that the problem under consideration is invariant under translations, for example, one may choose $\mathscr{R}_\lambda(\tau, x, \tau', x') = \lambda \mathrm{e}^{-(1-\lambda)(x-x')^2/\ell^2}$, where ℓ is a length scale at our disposal. Clearly, this choice does not only effectively limit the range of the interaction but also alters its functional form for $0 < \lambda < 1$ within the effective range defined by this function. Alternatively, one may therefore choose $\mathscr{R}_\lambda(\tau, x, \tau', x') = \lambda\theta(f_{\mathscr{R}}(\lambda) - (x - x')^2)$, where $f_{\mathscr{R}}(\lambda)$ is a (monotonous) function of dimension length squared with the constraints $f_{\mathscr{R}}(\lambda) \to 0$ for $\lambda \to 0$, $f_{\mathscr{R}}(\lambda) \to \infty$ for $\lambda \to 1$. Of course, other choices for the regulator function $\mathscr{R}_\lambda$ are also possible. Thus, if we think in terms of loop integrals constructed from density correlation functions, a suitably chosen regulator function can not only be used to switch on the interaction in the RG flow but also to specify the details of the momentum integrations in the loop integrals at a given value of λ. In all explicit calculations in this work, we shall always employ $\mathscr{R}_\lambda(\tau, x, \tau', x') = \lambda$ for simplicity. In any case, with respect to the RG equation for the energy density functional to be discussed below, we note that the result in the physical limit $\lambda \to 1$ does not depend on our choice for the regulator function, provided that we solve the RG equation for the energy density functional exactly.

The background potential confines the non-interacting fermions in the limit $\lambda = 0$. It should be chosen such that the initial non-interacting problem is simple to solve. In the examples discussed later in this work we will choose a potential V that describes a box with extent L, but other choices are also possible. For example, if one wants do describe interacting fermions in a harmonic trap, one chooses a harmonic potential. We emphasize that we only take into account a two-body interaction potential here. Higher-order many-body interactions will be dropped but can in principle be included straightforwardly in our DFT-RG approach.

Up to an irrelevant normalization factor, the generating functional Z_λ of the density correlation functions is given by

$$Z_\lambda[\{J_\sigma\}] \sim \int \mathscr{D}\psi^* \mathscr{D}\psi \, \mathrm{e}^{-S_\lambda[\psi^*,\psi] + \sum_\sigma \int_\tau \int_x J_\sigma(\tau,x)\,(\psi^*_\sigma(\tau,x)\psi_\sigma(\tau,x))} \equiv \mathrm{e}^{W_\lambda[J]}, \tag{3.3}$$

as discussed in Sec. 2.5. For convenience, we now shift the sources $\{J_\sigma\}$,

$$J_\sigma \to J_\sigma + \frac{1}{2} U_{\sigma\sigma}(0)\, \mathscr{R}_\lambda(\tau, x, \tau, x), \tag{3.4}$$

and then absorb this shift in a redefinition of the action S,

$$S \to S - \frac{1}{2} \sum_\sigma \int_\tau \int_x U_{\sigma\sigma}(0)\, \mathscr{R}_\lambda(\tau, x, \tau, x)\, \psi^*_\sigma(\tau, x) \psi_\sigma(\tau, x), \tag{3.5}$$

in the following. This shift bilinear in the fermion fields introduces an (additional) auxiliary background (one-body) potential into the problem. Taking into account the properties of the regulator function $\mathscr{R}_\lambda$, see Eq. (3.2), we observe that this redefinition of the action corresponds to a constant shift of the one-particle energies at the physical point $\lambda = 1$ and therefore yields nothing but a suitable normalization of the ground-state energy of the many-body system.

[1] Equivalently, instead of introducing a regulator function $\mathscr{R}_\lambda$, we may formally introduce a modified interaction $\tilde{U}_{2\mathrm{b},\lambda}$ in Eq. (3.1) which obeys the following conditions: $\lim_{\lambda\to 0} \tilde{U}_{2\mathrm{b},\lambda,\sigma\sigma'}(\tau, x, \tau', x') = 0$ and $\lim_{\lambda\to 1} \tilde{U}_{2\mathrm{b},\lambda,\sigma\sigma'}(\tau, x, \tau', x') = U_{2\mathrm{b},\sigma\sigma'}(\tau, x, \tau', x')$.

For our study of the dynamics of a system of N fermions, we also need to fix the particle numbers N_σ in our calculations. This can be either done by introducing chemical potentials into the action S or by choosing appropriate boundary conditions for the equations of motion [57]. In this work, we shall follow the latter approach to fix the particle number which amounts to fixing the particle number in the initial conditions for the RG flow equations of the density correlation functions. It can then be shown that the RG flow preserves the particle number as we shall discuss below.

From Eq. (3.3), we obtain the generating functional W_λ of the *connected* density correlation functions:

$$W_\lambda[\{J_\sigma\}] = \ln Z_\lambda[\{J_\sigma\}]\,. \tag{3.6}$$

This functional can be expanded in terms of the sources $\{J_\sigma\}$:

$$\begin{aligned} W_\lambda[\{J_\sigma\}] = G_\lambda^{(0)} &+ \sum_\sigma \int_\tau \int_x G^{(1)}_{\lambda,\sigma}(\tau,x)\, J_\sigma(\tau,x) \\ &+ \sum_{\sigma_1\sigma_2} \frac{1}{2} \int_{\tau_1} \int_{x_1} \int_{\tau_2} \int_{x_2} G^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1,x_1,\tau_2,x_2)\, J_{\sigma_1}(\tau_1,x_1)\, J_{\sigma_2}(\tau_2,x_2) + \dots\,, \end{aligned} \tag{3.7}$$

where $G_\lambda^{(0)} = W_\lambda[0]$ is related to the ground-state energy of the system. The quantity

$$\rho_{\mathrm{gs},\lambda,\sigma}(\tau,x) := G^{(1)}_{\lambda,\sigma}(\tau,x) = \left.\frac{\delta W_\lambda[\{J_\sigma\}]}{\delta J_\sigma(\tau,x)}\right|_{J_\sigma=0} \tag{3.8}$$

is the time-dependent ground-state (gs) density, and

$$G^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1,x_1,\tau_2,x_2) = \left.\frac{\delta^2 W_\lambda[\{J_\sigma\}]}{\delta J_{\sigma_1}(\tau_1,x_1)\,\delta J_{\sigma_2}(\tau_2,x_2)}\right|_{J_\sigma=0} \tag{3.9}$$

is the fully time-dependent density-density correlation function. The n-density correlation functions

$$G^{(n)}_{\lambda,\sigma_1\dots\sigma_n}(\tau_1,x_1,\dots,\tau_n,x_n) = \left.\frac{\delta^n W_\lambda[\{J_\sigma\}]}{\delta J_{\sigma_1}(\tau_1,x_1)\cdots\delta J_{\sigma_n}(\tau_n,x_n)}\right|_{J_\sigma=0} \tag{3.10}$$

can in principle be computed from the one-particle propagators. We shall exploit this below to compute the initial conditions for the RG flow equations. Note that, even for the non-interacting system, all density correlation functions $G^{(n)}_{\lambda,\sigma_1\dots\sigma_n}$ are in general finite which reflects the well-known fact that even the energy density functional of a non-interacting system represents a non-local functional.

For convenience, we define the time-independent ground-state density $n_{\mathrm{gs},\lambda,\sigma}(x)$ as follows:

$$n_{\mathrm{gs},\lambda,\sigma}(x) := \lim_{\beta\to\infty} \frac{1}{\beta} \int_{-\beta/2}^{\beta/2} \mathrm{d}\tau\, \rho_{\mathrm{gs},\lambda,\sigma}(\tau,x), \tag{3.11}$$

where β is an auxiliary parameter introduced to define a finite imaginary time interval, $\tau \in [-\beta/2, \beta/2)$. In our numerical calculations, we shall always consider the case $\beta \to \infty$, i. e. $\tau \in (-\infty, \infty)$. In any case, if the density $\rho_{\mathrm{gs},\lambda,\sigma}(\tau,x)$ turns out to be independent of the imaginary time τ, then we have $n_{\mathrm{gs},\lambda,\sigma}(x) \equiv \rho_{\mathrm{gs},\lambda,\sigma}(\tau,x)$. For instantaneous interactions as used in the present work, this is indeed the case.

Next, we introduce the so-called *classical* fields $\{\rho_\sigma(\tau,x)\}$:

$$\rho_\sigma(\tau,x) = \frac{\delta W_\lambda[\{J_\sigma\}]}{\delta J_\sigma(\tau,x)}\,. \tag{3.12}$$

The classical fields $\{\rho_\sigma\}$ are related to the fermion densities, see Eq. (3.8), and plays the role of a composite bosonic effective degree of freedom in our approach which is used to describe the dynamics of fermions. Note that $\{\rho_\sigma\}$ are also functionals of the sources $\{J_\sigma\}$, $\rho_\sigma = \rho_\sigma[\{J_\sigma\}]$, and that, in our case, it also depends on λ. Here, we do not indicate this dependence explicitly (e. g., by adding an index λ) to ensure that this quantity is not confused with the actual λ-dependent ground-state density. However, we need to keep the λ-dependence in mind for the derivation of the flow equation of the energy density functional below.

The 2PPI effective action $\Gamma_\lambda[\{\rho_\sigma\}]$ is now obtained from a Legendre transformation of the functional $W[\{J_\sigma\}]$ with respect to the sources $\{J_\sigma\}$:

$$\Gamma_\lambda[\{\rho_\sigma\}] = \sup_{\{J_\sigma\}} \left\{ -W_\lambda[\{J_\sigma\}] + \sum_\sigma \int_\tau \int_x J_\sigma(\tau,x)\, \rho_\sigma(\tau,x) \right\}. \tag{3.13}$$

Below we shall consider an expansion of Γ_λ in terms of λ-independent classical fields $\{\rho_\sigma\}$. From Eq. (3.13), we then deduce that the sources $J_\sigma = J_{\sigma,\mathrm{sup}}$, which fulfill the supremum condition, depend on λ and are functionals of $\{\rho_\sigma\}$, i. e. $J_{\sigma,\mathrm{sup}} = J_{\sigma,\mathrm{sup}}[\{\rho_\sigma\}]$. Phenomenologically, this transformation to the 2PPI effective action may be viewed as a bosonization of the theory since we have traded in the fermion fields in the classical action S for the composite bosonic fields $\{\rho_\sigma\}$ in the effective action Γ_λ.

The 2PPI effective action Γ_λ can be related to the energy-density functional, see Eq. (2.54). Along the lines detailed in Sec. 2.5, we can also define the relations for the λ-dependent properties. For the λ-dependent ground-state energy E_λ for example, we find

$$E_\lambda = \lim_{\beta\to\infty} \frac{1}{\beta} \Gamma_\lambda[\{\rho_{\mathrm{gs},\sigma}\}] = -\lim_{\beta\to\infty} \frac{1}{\beta} W_\lambda[0], \tag{3.14}$$

and the λ-dependent quantum equation of motion of the composite degree of freedom ρ reads

$$\frac{\delta\Gamma_\lambda[\{\rho_\sigma\}]}{\delta\rho_\sigma(\tau,x)} = J_\sigma(\tau,x). \tag{3.15}$$

The solution of this equation yields the ground-state density $\rho_{\mathrm{gs},\lambda,\sigma}$ of the system in the limit $J_\sigma \to 0$.

As mentioned in the previous chapter, in conventional DFT often a global ansatz for the *a priori* unknown energy density functional is made. This ansatz is then minimized using the famous *Kohn-Sham* equations, see Sec. 2.3. Here, we refrain from making a global ansatz for the density functional but follow the approach detailed in Ref. [22] and expand Γ_λ about its ground state $\rho_{\mathrm{gs},\lambda,\sigma}$:

$$\Gamma_\lambda[\{\rho_\sigma\}] = \Gamma_\lambda[\{\rho_{\mathrm{gs},\lambda,\sigma}\}] + \frac{1}{2} \sum_{\sigma_1\sigma_2} \int_{\chi_1} \int_{\chi_2} \left(\rho_{\sigma_1}(\chi_1) - \rho_{\mathrm{gs},\lambda,\sigma_1}(\chi_1)\right) \Gamma^{(2)}_{\lambda,\sigma_1\sigma_2}(\chi_1,\chi_2) \left(\rho_{\sigma_2}(\chi_2) - \rho_{\mathrm{gs},\lambda,\sigma_2}(\chi_2)\right) + \ldots. \tag{3.16}$$

For convenience, we have introduced $\chi = \{\tau, x\}$, $\int_\chi = \int_{-\infty}^{\infty} \mathrm{d}\tau \int_{-\infty}^{\infty} \mathrm{d}x$, and

$$\Gamma^{(2)}_{\lambda,\sigma_1\sigma_2}(\chi_1,\chi_2) = \left. \frac{\delta^2\Gamma_\lambda[\{\rho_\sigma\}]}{\delta\rho_{\sigma_1}(\chi_1)\,\delta\rho_{\sigma_2}(\chi_2)} \right|_{\rho_\sigma=\rho_{\mathrm{gs},\sigma}} \tag{3.17}$$

is positive definite by construction.

Clearly, the expansion of W_λ in terms of $\{J_\sigma\}$ and the expansion of Γ_λ in terms of $\{\rho_\sigma\}$ are related. From Eq. (3.8), we deduce that the ground-state density $\rho_{\mathrm{gs},\lambda,\sigma}$ and the one-density correlation function $G^{(1)}_{\lambda,\sigma}$ are equivalent. From

Eqs. (3.12) and (3.15), it moreover follows that the "curvature" $\Gamma^{(2)}_{\lambda,\sigma_1\sigma_2}$ is related to the density-density correlation function $G^{(2)}_{\lambda,\sigma_1\sigma_2}$ appearing in the expansion (3.7). In fact, we have

$$\frac{\delta^2\Gamma_\lambda[\{\rho_\sigma\}]}{\delta\rho_{\sigma_1}(\chi_1)\delta\rho_{\sigma_2}(\chi_2)} = \left(\frac{\delta^2 W_\lambda[\{J_\sigma\}]}{\delta J\,\delta J}\right)^{-1}_{\sigma_1\sigma_2}(\chi_1,\chi_2) \tag{3.18}$$

and therefore it follows that

$$\Gamma^{(2)}_{\lambda,\sigma_1\sigma_2}(\chi_1,\chi_2) = \left(G^{(2)}_\lambda\right)^{-1}_{\sigma_1\sigma_2}(\chi_1,\chi_2). \tag{3.19}$$

Corresponding relations for density correlation functions of higher order can be derived along these lines. For the three-density correlation function, for example, we find

$$\frac{\delta^3\Gamma_\lambda[\{\rho_\sigma\}]}{\delta\rho_{\sigma_1}(\chi_1)\delta\rho_{\sigma_2}(\chi_2)\delta\rho_{\sigma_3}(\chi_3)} = \frac{\delta}{\delta\rho_{\sigma_3}(\chi_3)}\left(\frac{\delta^2 W_\lambda[\{J_\sigma\}]}{\delta J\,\delta J}\right)^{-1}_{\sigma_1\sigma_2}(\chi_1,\chi_2), \tag{3.20}$$

which yields

$$\Gamma^{(3)}_{\lambda,\sigma_1\sigma_2\sigma_3}(\chi_1,\chi_2,\chi_3) = -\sum_{\sigma_4\sigma_5\sigma_6}\int_{\chi_4}\int_{\chi_5}\int_{\chi_6}\left(\Gamma^{(2)}_{\lambda,\sigma_1\sigma_4}(\chi_1,\chi_4)\,G^{(3)}_{\lambda,\sigma_4\sigma_5\sigma_6}(\chi_4,\chi_5,\chi_6)\,\Gamma^{(2)}_{\lambda,\sigma_5\sigma_2}(\chi_5,\chi_2)\,\Gamma^{(2)}_{\lambda,\sigma_6\sigma_3}(\chi_6,\chi_3)\right), \tag{3.21}$$

where

$$\Gamma^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}(\chi_1,\chi_2,\ldots,\chi_n) = \left.\frac{\delta^n\Gamma_\lambda[\{\rho_\sigma\}]}{\delta\rho_{\sigma_1}(\chi_1)\cdots\delta\rho_{\sigma_n}(\chi_n)}\right|_{\rho_\sigma=\rho_{\mathrm{gs},\sigma}}. \tag{3.22}$$

For later purposes, we finally provide the relation between $G^{(4)}_{\lambda,\sigma_1\ldots\sigma_4}$ and $\Gamma^{(4)}_{\lambda,\sigma_1\ldots\sigma_4}$:

$$\begin{aligned}
&\Gamma^{(4)}_{\lambda,\sigma_1\sigma_2\sigma_3\sigma_4}(\chi_1,\chi_2,\chi_3,\chi_4)\\
&= -\sum_{\sigma_5\sigma_6\sigma_7}\int_{\chi_5}\int_{\chi_6}\int_{\chi_7}\Big(\Gamma^{(3)}_{\lambda,\sigma_1\sigma_5\sigma_4}(\chi_1,\chi_5,\chi_4)\,G^{(3)}_{\lambda,\sigma_5\sigma_6\sigma_7}(\chi_5,\chi_6,\chi_7)\,\Gamma^{(2)}_{\lambda,\sigma_6\sigma_2}(\chi_6,\chi_2)\,\Gamma^{(2)}_{\lambda,\sigma_7\sigma_3}(\chi_7,\chi_3)\\
&\qquad + \Gamma^{(2)}_{\lambda,\sigma_1\sigma_5}(\chi_1,\chi_5)\,G^{(3)}_{\lambda,\sigma_5\sigma_6\sigma_7}(\chi_5,\chi_6,\chi_7)\,\Gamma^{(3)}_{\lambda,\sigma_6\sigma_2\sigma_4}(\chi_6,\chi_2,\chi_4)\,\Gamma^{(2)}_{\lambda,\sigma_7\sigma_3}(\chi_7,\chi_3)\\
&\qquad + \Gamma^{(2)}_{\lambda,\sigma_1\sigma_5}(\chi_1,\chi_5)\,G^{(3)}_{\lambda,\sigma_5\sigma_6\sigma_7}(\chi_5,\chi_6,\chi_7)\,\Gamma^{(2)}_{\lambda,\sigma_6\sigma_2}(\chi_6,\chi_2)\,\Gamma^{(3)}_{\lambda,\sigma_7\sigma_3\sigma_4}(\chi_7,\chi_3,\chi_4)\Big)\\
&\quad - \sum_{\sigma_5\ldots\sigma_8}\int_{\chi_5}\int_{\chi_6}\int_{\chi_7}\int_{\chi_8}\Gamma^{(2)}_{\lambda,\sigma_1\sigma_5}(\chi_1,\chi_5)\,G^{(4)}_{\lambda,\sigma_5\sigma_6\sigma_7\sigma_8}(\chi_5,\chi_6,\chi_7,\chi_8)\,\Gamma^{(2)}_{\lambda,\sigma_6\sigma_2}(\chi_6,\chi_2)\,\Gamma^{(2)}_{\lambda,\sigma_7\sigma_3}(\chi_7,\chi_3)\,\Gamma^{(2)}_{\lambda,\sigma_8\sigma_4}(\chi_8,\chi_4).
\end{aligned} \tag{3.23}$$

Thus, general correlation functions $\Gamma^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$ can be obtained from a computation of the (connected) density correlation functions $G^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$. The computation of these functions for an interacting theory (i. e., for $\lambda > 0$) is in general highly non-trivial and will be discussed below within our DFT-RG framework which only uses the density correlation functions of the non-interacting theory as an input. The latter can be computed from the one-particle propagator $\Delta_{0,\sigma}$ of the non-interacting theory,

$$\begin{aligned}
\Delta_{0,\sigma}(\tau_1,x_1,\tau_2,x_2) &= -\langle\mathcal{T}\psi_\sigma(\tau_1,x_1)\,\psi^*_\sigma(\tau_2,x_2)\rangle\\
&= -\langle\psi_\sigma(\tau_1,x_1)\,\psi^*_\sigma(\tau_2,x_2)\rangle\,\theta_\tau(\tau_1-\tau_2) + \langle\psi^*_\sigma(\tau_2,x_2)\,\psi_\sigma(\tau_1,x_1)\rangle\,\theta_\tau(\tau_2-\tau_1),
\end{aligned} \tag{3.24}$$

where $\mathcal{T}$ is the time-ordering operator. Here, $\theta_\tau(\tau) = 1$ for $\tau > 0$ as well as for $\tau \to 0^+$ and $\theta_\tau(\tau) = 0$ otherwise. The non-interacting ground-state density is then obtained from

$$\rho_{\mathrm{gs},\lambda=0,\sigma_1}(\tau_1, x_1) \equiv G^{(1)}_{\lambda=0,\sigma_1}(\tau_1, x_1) = \lim_{\tau_2 \to \tau_1^+} \Delta_{0,\sigma_1}(\tau_1, x_1, \tau_2, x_1)\,. \tag{3.25}$$

Higher-order density correlation functions can be written as expectation values of time-ordered products of the fields as well. In fact, the general n-density correlation functions $Z^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$ including both connected and disconnected diagrams are defined as follows:

$$Z^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}(\chi_1,\ldots,\chi_n) = \langle \mathcal{T}\psi^*_{\sigma_1}(\chi_1)\psi_{\sigma_1}(\chi_1)\cdots\psi^*_{\sigma_n}(\chi_n)\psi_{\sigma_n}(\chi_n)\rangle_\lambda\,, \tag{3.26}$$

where $Z^{(1)}_{\lambda,\sigma} \equiv G^{(1)}_{\lambda,\sigma}$ and the index λ refers to the fact that the expectation value has to be computed with respect to the λ-dependent ground state. Using the *Wick* theorem, the (connected) density correlation functions $G^{(n)}_{\lambda=0,\sigma_1\ldots\sigma_n}$ of the non-interacting theory can be extracted from the correlation functions $Z^{(n)}_{\lambda=0,\sigma_1\ldots\sigma_n}$ and can then be written in terms of one-particle propagators. For the connected density-density correlation function, we find

$$Z^{(2)}_{\lambda,\sigma_1\sigma_2}(\chi_1,\chi_2) = \rho_{\mathrm{gs},\lambda,\sigma_1}(\chi_1)\rho_{\mathrm{gs},\lambda,\sigma_2}(\chi_2) + G^{(2)}_{\lambda,\sigma_1\sigma_2}(\chi_1,\chi_2) \tag{3.27}$$

with

$$G^{(2)}_{\lambda=0,\sigma_1\sigma_2}(\chi_1,\chi_2) = \begin{cases} -\Delta_{0,\sigma_1}(\chi_2,\chi_1)\,\Delta_{0,\sigma_1}(\chi_1,\chi_2) & \text{for } \sigma_1 = \sigma_2\,, \\ 0 & \text{for } \sigma_1 \neq \sigma_2\,. \end{cases} \tag{3.28}$$

It follows from Eq. (3.24) that $G^{(2)}_{\lambda=0,\sigma_1\sigma_2}$ only depends on $|\tau_1 - \tau_2|$. For $\lambda = 0$ the density-density correlation function $G^{(2)}_{\lambda=0,\sigma_1\sigma_2}$ is zero when the spin-indices are not equal, because in this non-iteracting limit there is no correlation between the different spin species. Therefore, we introduce the short-hand notation:

$$G^{(2)}_{\lambda=0,\sigma}(\chi_1,\chi_2) \equiv G^{(2)}_{\lambda=0,\sigma\sigma}(\chi_1,\chi_2) \tag{3.29}$$

for the case of equal spin-indices. In the case of higher-order density correlation functions also only the correlation functions with equal spin-indices are non-zero and we introduce the short-hand notation:

$$G^{(n)}_{\lambda=0,\sigma}(\chi_1,\ldots,\chi_n) \equiv G^{(n)}_{\lambda=0,\sigma\ldots\sigma}(\chi_1,\ldots,\chi_n) \tag{3.30}$$

for the $\lambda = 0$ limit. For the three-density correlation function $G^{(3)}_{\lambda=0,\sigma}$ with three equal spin indices, we obtain

$$G^{(3)}_{\lambda=0,\sigma}(\chi_1,\chi_2,\chi_3) = \Delta_{0,\sigma}(\chi_1,\chi_2)\,\Delta_{0,\sigma}(\chi_2,\chi_3)\,\Delta_{0,\sigma}(\chi_3,\chi_1) + \Delta_{0,\sigma}(\chi_2,\chi_1)\,\Delta_{0,\sigma}(\chi_1,\chi_3)\,\Delta_{0,\sigma}(\chi_3,\chi_2)\,. \tag{3.31}$$

The four-density correlation function $G^{(4)}_{\lambda=0,\sigma}$ with four equal spin indices, entering the computation of the expansion coefficient $\Gamma^{(4)}_{\lambda=0,\sigma_1\ldots\sigma_4}$, can be written as follows:

$$\begin{aligned} G^{(4)}_{\lambda=0,\sigma}(\chi_1,\ldots,\chi_4) = &-\Delta_{0,\sigma}(\chi_1,\chi_2)\,\Delta_{0,\sigma}(\chi_2,\chi_3)\,\Delta_{0,\sigma}(\chi_3,\chi_4)\,\Delta_{0,\sigma}(\chi_4,\chi_1) \\ &-\Delta_{0,\sigma}(\chi_1,\chi_4)\,\Delta_{0,\sigma}(\chi_4,\chi_3)\,\Delta_{0,\sigma}(\chi_3,\chi_2)\,\Delta_{0,\sigma}(\chi_2,\chi_1) \\ &-\Delta_{0,\sigma}(\chi_2,\chi_4)\,\Delta_{0,\sigma}(\chi_4,\chi_3)\,\Delta_{0,\sigma}(\chi_3,\chi_1)\,\Delta_{0,\sigma}(\chi_1,\chi_2) \\ &-\Delta_{0,\sigma}(\chi_1,\chi_4)\,\Delta_{0,\sigma}(\chi_4,\chi_2)\,\Delta_{0,\sigma}(\chi_2,\chi_3)\,\Delta_{0,\sigma}(\chi_3,\chi_1) \\ &-\Delta_{0,\sigma}(\chi_2,\chi_4)\,\Delta_{0,\sigma}(\chi_4,\chi_1)\,\Delta_{0,\sigma}(\chi_1,\chi_3)\,\Delta_{0,\sigma}(\chi_3,\chi_2) \\ &-\Delta_{0,\sigma}(\chi_3,\chi_4)\,\Delta_{0,\sigma}(\chi_4,\chi_2)\,\Delta_{0,\sigma}(\chi_2,\chi_1)\,\Delta_{0,\sigma}(\chi_1,\chi_3)\,. \end{aligned} \tag{3.32}$$

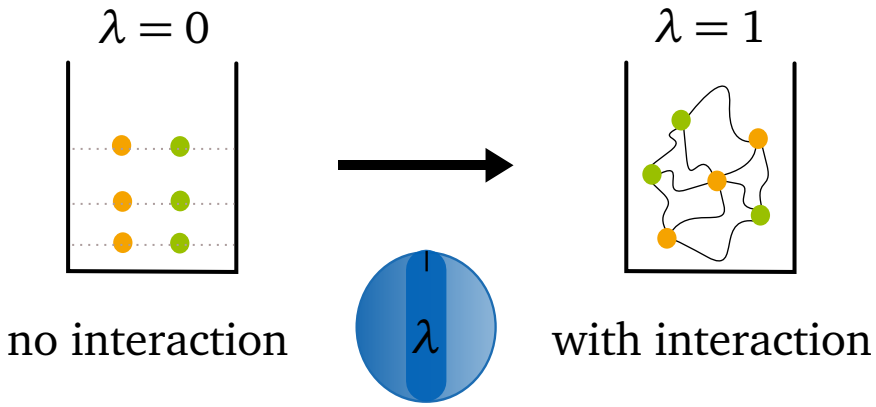

Figure 3.1.: Schematic illustration of the transition from the initial condition associated with the non-interacting system at $\lambda = 0$ to the interacting system at $\lambda = 1$. The flow equation interpolates between the two systems.

Higher-order correlation functions can be computed along these lines. We find

$$G^{(n)}_{\lambda=0,\sigma}(\chi_1,\ldots,\chi_n) = \frac{(-1)^{n+1}}{n} \sum_{(i_1,\ldots,i_n)\in S_n} \Delta_{0,\sigma}(\chi_{i_1},\chi_{i_2})\Delta_{0,\sigma}(\chi_{i_2},\chi_{i_3})\cdots\Delta_{0,\sigma}(\chi_{i_{n-1}},\chi_{i_n})\Delta_{0,\sigma}(\chi_{i_n},\chi_1), \tag{3.33}$$

where S_n is the set of all permutations of the n-tuple $(1,2,\ldots,n)$. In our explicit calculations discussed below, however, we shall only take into account n-density correlation functions with $n \leq 4$.

Let us now come to the derivation of a flow equation for the density functional Γ_λ, taking into account the full time-dependence of the correlation functions. Our discussion already makes apparent that the computation of Γ_λ can be traced back to the computation of density correlation functions. In the non-interacting limit, i. e. $\lambda = 0$, these functions can be calculated analytically for a large class of confining geometries. This defines the initial point of our RG flow and we will discuss the computation of the initial conditions for our system in more detail below. In the fully interacting limit, i. e. $\lambda = 1$, the correlation functions cannot be computed straightforwardly. However, we can derive exact equations for the computation of the change of the generating functional W_λ and the density functional Γ_λ under a variation of λ. In Fig. 3.1 a schematic illustration of this flow is shown. To this end, we consider Eq. (3.6) and take the derivative of W_λ with respect to λ. This yields

$$\begin{aligned}
&\partial_\lambda W_\lambda[\{J_\sigma\}] \\
&\quad = -\frac{1}{2}\int_{\chi_1}\int_{\chi_2} \frac{\delta W_\lambda[\{J_\sigma\}]}{\delta J_{\sigma_1}(\chi_1)} U_{2\mathrm{b},\sigma_1\sigma_2}(\chi_1,\chi_2)\,(\partial_\lambda \mathscr{R}_\lambda(\chi_1,\chi_2))\,\frac{\delta W_\lambda[\{J_\sigma\}]}{\delta J_{\sigma_2}(\chi_2)} \\
&\qquad -\frac{1}{2}\int_{\chi_1}\int_{\chi_2} U_{2\mathrm{b},\sigma_1\sigma_2}(\chi_1,\chi_2)\,(\partial_\lambda \mathscr{R}_\lambda(\chi_1,\chi_2))\left(\frac{\delta^2 W_\lambda[\{J_\sigma\}]}{\delta J_{\sigma_2}(\chi_2)\delta J_{\sigma_1}(\chi_1)} - \frac{\delta W_\lambda[\{J_\sigma\}]}{\delta J_{\sigma_2}(\chi_2)}\,\delta_{\sigma_1\sigma_2}\,\delta(\chi_2-\chi_1)\right),
\end{aligned} \tag{3.34}$$

where $\partial_\lambda = \frac{\partial}{\partial\lambda}$ and $\delta(\chi_1-\chi_2) \equiv \delta(\tau_1-\tau_2)\delta(x_1-x_2)$. This equation is exact on the level of two-body interactions and allows to compute the change of the functional $W_\lambda[\{J_\sigma\}]$ under a variation of λ. The initial condition for this differential equation is given by the non-interacting system associated with $\lambda = 0$. The fully interacting many-body problem is obtained in the limit $\lambda = 1$. While this flow equation is exact, its solution in general requires approximations, as its right-hand side depends on functional derivatives of W_λ with respect to the sources $\{J_\sigma\}$. To solve this equation in a systematic fashion, we insert the expansion (3.7) of the functional W_λ into Eq. (3.34). This allows us to derive flow equations for the density correlation functions $G^{(n)}_\lambda$ by comparing the same orders in $\{J_\sigma\}$ on the left- and right-hand side of Eq. (3.34). The flow equations for the energy, the density and the density correlation functions can be found in Sec. 3.3. In Sec. 3.4, we shall then show that such an expansion is indeed systematic in the sense that it can be systematically related to many-body perturbation theory. Nevertheless, our approach

is non-perturbative. The solutions $G^{(n)}_{\lambda=1,\sigma_1\ldots\sigma_n}$ of these flow equations rather contain arbitrarily high orders in the coupling constant associated with a perturbative calculation. We also emphasize that the expansion (3.7) yields an infinite tower of coupled flow equations for the correlation functions $G^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$. From Eq. (3.34), we deduce that the flow equation for $G^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$ in general depends on the correlation functions $G^{(m)}_{\lambda,\sigma_1\ldots\sigma_m}$ with $1 \leq m \leq n+2$. This suggests that a truncation of this set of equations is in general required in order to compute the density correlation functions. Below, we shall discuss the truncation scheme underlying our present studies in more detail. In any case, the correlation functions $G^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$ obtained from a solution of such a (truncated) set of flow equations can be used to compute the functions $\Gamma^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$ determining the density functional Γ_λ. As we have discussed above, the functionals W_λ and Γ_λ are related via a Legendre transformation. Using the flow equation (3.34) for the generating functional of the connected correlation functions and the definition (3.13) of the density functional Γ_λ, we find the following flow equation for Γ_λ:

$$\begin{aligned}
&\partial_\lambda \Gamma_\lambda[\{\rho_\sigma\}] \\
&\quad = \frac{1}{2}\int_{\chi_1}\int_{\chi_2} \rho_{\sigma_1}(\chi_1)\, U_{2\mathrm{b},\sigma_1\sigma_2}(\chi_1,\chi_2)\, (\partial_\lambda \mathscr{R}_\lambda(\chi_1,\chi_2))\, \rho_{\sigma_2}(\chi_2) \\
&\quad + \frac{1}{2}\int_{\chi_1}\int_{\chi_2} U_{2\mathrm{b},\sigma_1\sigma_2}(\chi_1,\chi_2)\, (\partial_\lambda \mathscr{R}_\lambda(\chi_1,\chi_2)) \left(\left(\frac{\delta^2 \Gamma_\lambda[\{\rho_\sigma\}]}{\delta\rho\, \delta\rho} \right)^{-1}_{\sigma_1\sigma_2} (\chi_2,\chi_1) - \rho_{\sigma_2}(\chi_2)\, \delta_{\sigma_1\sigma_2}\, \delta(\chi_2-\chi_1) \right). \quad (3.35)
\end{aligned}$$

This functional differential equation is again *exact* on the level of two-body interactions and describes the flow of the density functional from the non-interacting system at the initial point $\lambda = 0$ to the fully interacting many-body system at $\lambda = 1$. The flow equations for W_λ and Γ_λ look indeed quite similar. However, we would like to stress that the fundamental building blocks of these flow equations, i. e. the correlation functions, are not identical. Whereas the connected density correlation functions enter the flow of the functional W_λ, 2PPI correlation functions underly the flow of the density functional Γ_λ. Of course, these correlation functions can be translated into each other, as shown explicitly in Eqs. (3.19), (3.21), and (3.23).

We observe that the flow equation (3.35) for the 2PPI effective action has a simple so-called one-loop structure as is the case for the RG flow equation for the one-particle irreducible (1PI) effective action derived by Wetterich [58]. As already indicated in the case of the flow equation for W_λ, however, this does by no means imply that only one-loop corrections are taken into account with this flow equation. In fact, by solving the functional differential equation (3.35), we automatically include arbitrarily high orders in a loop expansion. Moreover, we emphasize that the derivation of this flow equation does not require that the interaction strength is small.

In terms of the terminology of many-body physics, the first term on the right-hand side of Eq. (3.35) (and analogously of Eq. (3.34)) can be identified with the *Hartree* term, see also the discussion in Sec. 3.5. The second term on the right-hand side contains all other contributions, including *Fock* contributions as we shall discuss in more detail in Sec. 6.3. Moreover, we would like to stress that the expansion (3.16) of the density functional about the ground state is an exact expansion and should by no means be confused with the local density approximation. This is already clear from the fact that the $\Gamma^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$ functions, which determine the functional Γ_λ, depend on the imaginary time and the spatial coordinates, see also our discussion of the relation of our approach to conventional DFT in Sec. 3.6.

As in the case of the flow equation for W_λ, also the flow equation (3.35) for the density functional can in general not be solved exactly. To construct systematically the exact solution of this equation, we can make use of the expansion (3.16) about the ground state ρ_{gs}. Plugging this expansion into the general flow equation (3.35) and comparing the same orders in $(\rho - \rho_{\mathrm{gs}})$ on the left- and right-hand side, we obtain flow equations for the 2PPI correlation functions $\Gamma^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$. In complete analogy to the flow equations for the connected correlation functions, this yields an infinite tower of coupled differential equations for the 2PPI correlation functions. To be more specific, the flow of the $\Gamma^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$ function for $n \geq 2$ in general depends on $\Gamma^{(m)}_{\lambda,\sigma_1\ldots\sigma_m}$ with $2 \leq m \leq n+2$. As we expand about the ground state, the flow equation for the $\Gamma^{(1)}_{\lambda,\sigma}$ function vanishes by construction.

The flow equations (3.34) and (3.35) are equivalent on a formal level. However, the computation of the initial conditions of the 2PPI correlation functions require an inversion of the density-density correlation function $G^{(2)}_{\lambda,\sigma_1\sigma_2}$. The latter can be derived conveniently from the one-particle propagator, see Eq. (3.28). While the inversion of this correlation function may be simple for theories which are invariant under translation in time and space, it may turn out to be highly involved in any other case, such as fermions trapped in a harmonic potential. Moreover, the computation of the initial conditions for the $\Gamma^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$ functions is tedious in general, as can be seen from Eqs. (3.19), (3.21), and (3.23), and always requires the connected density correlators $G^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$ as an input. Therefore, we shall consider the flow equation (3.34) from here on for any explicit calculation. As stated above, the resulting connected density correlation functions can in principle be used to construct the density functional Γ_λ, if needed.

We close this section by commenting briefly on the RG philosophy underlying our approach which is of the *Callan-Symanzik* type. Originally, *Callan* and *Symanzik* aimed at a study of the scaling behavior of correlation functions under a variation of the renormalized mass in relativistic field theories [59, 60, 61]. Indeed, the famous *Callan-Symanzik* equation follows from taking the derivative of the one-particle irreducible n-point correlation function with respect to the (renormalized) mass. This yields a set of differential equations which allows to study the scaling behavior of the correlation functions, e. g., in the limit of small masses or, equivalently, large momenta. In other words, this type of RG equation follows from taking the derivative of correlation functions with respect to a suitably chosen parameter/coupling associated with a term bilinear in the fields in the underlying action, e. g., the mass parameter in the case of the *Callan-Symanzik* equation. In our case, we rescale the two-body interaction with a dimensionless control parameter λ and study then the change of the correlation functions under a variation of this parameter. Here, we assume $\mathscr{R}_\lambda = \lambda$ for the regulator function. The RG equations for these functions follow from taking the derivative of the generating functional of either the connected correlation functions or the 2PPI correlation functions with respect to λ and describe the change of these functions under a (specific) variation of the two-body interaction. Alternatively, if we bosonized the action (3.1) already on the level of the path integral by employing a *Hubbard-Stratonovich* transformation to introduce an (auxiliary) composite field $\rho_\sigma(\tau,x) \sim \psi^*_\sigma(\tau,x)\psi_\sigma(\tau,x)$, the two-body interaction would appear in a term bilinear in the auxiliary field ρ_σ and, in the spirit of the *Callan-Symanzik* equation, may be viewed as a λ-dependent non-local (mass-like) gap for the fields $\{\rho_\sigma\}$. The variation of this term with respect to λ in the *Hubbard-Stratonovich*-transformed theory, which is still equivalent to the original theory, then allows us in principle again to compute the behavior of the correlation functions as a function of the control parameter λ, making the analogy to the *Callan-Symanzik* approach even more apparent.

3.2 Density-Density Correlation Function and Spectral Function

Let us now discuss some properties of the density correlation functions, with an emphasis on the density-density correlation function.

Loosely speaking, the density correlation functions $G^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$ are related to the probability to find a fermion with spin σ_1 at, e. g., a given point x_1 and the other fermions with a given spin configuration at $x_2,\ldots,x_N$. For example, the spin-σ density is related to the probability to find a fermion with spin σ at point x:

$$n_{\mathrm{gs},\lambda,\sigma}(x) \equiv \rho_{\mathrm{gs},\lambda,\sigma}(0,x) = \langle \psi^*_\sigma(0,x)\,\psi_\sigma(0,x)\rangle_\lambda\,. \tag{3.36}$$

Here, we have used Eq. (3.25), which is also valid for finite λ, and assumed that we are only considering theories which are time-translation invariant. This allows us to set $\tau = 0$ without loss of generality. The total density is related to the probability to find a fermion with any spin at point x:

$$n_{\mathrm{gs},\lambda}(x) \equiv \rho_{\mathrm{gs},\lambda}(0,x) = \sum_\sigma \langle \psi^*_\sigma(0,x)\,\psi_\sigma(0,x)\rangle_\lambda\,, \tag{3.37}$$

where the density $n_{\mathrm{gs},\lambda}$ is the sum over the spin-densities $n_{\mathrm{gs},\lambda,\sigma}$,

$$n_{\mathrm{gs},\lambda}(x) = \sum_{\sigma} n_{\mathrm{gs},\lambda,\sigma}(x)\,. \tag{3.38}$$

From an integration of the density $n_{\mathrm{gs},\lambda,\sigma}(x)$ with respect to x, we then obtain N_σ, the number of fermions with spin σ, and from an integration of the density $n_{\mathrm{gs},\lambda}(x)$ with respect to x we obtain the total number of fermions, $N = \sum_\sigma N_\sigma$.

We would also like to calculate the spin-σ density in the operator formalism. Therefore we define the spin-σ density operator

$$\hat{n}_\sigma(x) = \sum_{i\in\mathscr{M}_\sigma} \delta(x-\hat{x}_i)\,, \quad \text{with} \quad \mathscr{M}_\sigma = \{i\,|\sigma_i = \sigma\} \quad \text{and} \quad |\mathscr{M}_\sigma| = N_\sigma\,. \tag{3.39}$$

The system under consideration has a defined number N_σ of fermions with spin σ and thereby the spin configuration is defined. Since the total square of the wavefunction is invariant under an exchange of the parameter pairs (x_i,σ_i), e. g. $|\Psi_{\mathrm{gs},\lambda}(x_1,\sigma_1,x_2,\sigma_2,\ldots,x_N,\sigma_N)|^2 = |\Psi_{\mathrm{gs},\lambda}(x_2,\sigma_2,x_1,\sigma_1,\ldots,x_N,\sigma_N)|^2$, we can always rearrange the order of the parameter pairs such that a set (x_i,σ_i) appears as the first argument, as long as we do not change the number of fermions with a particular spin. For the spin-σ density we find

$$\begin{aligned} n_{\mathrm{gs},\lambda,\sigma}(x) &= \langle\Psi_{\mathrm{gs},\lambda}|\hat{n}_\sigma(x)|\Psi_{\mathrm{gs},\lambda}\rangle \\ &= N_\sigma \int_{x_2}\cdots\int_{x_N} |\Psi_{\mathrm{gs},\lambda}(x,\sigma,x_2,\sigma_2,\ldots,x_N,\sigma_N)|^2\,, \end{aligned} \tag{3.40}$$

where $|\Psi_{\mathrm{gs},\lambda}\rangle$ (with $\langle\Psi_{\mathrm{gs},\lambda}|\Psi_{\mathrm{gs},\lambda}\rangle = 1$) denotes the ground-state wavefunction. Note that the spin indices $\sigma_2,\ldots,\sigma_N$ are no free parameters but, up to changes in the order of the indices, fixed by the definition of the system under consideration.

Correspondingly, the correlation function $Z^{(2)}_{\lambda,\sigma_1\sigma_2}$ evaluated at $\tau_1 = \tau_2$,

$$Z^{(2)}_{\lambda,\sigma_1\sigma_2}(0,x_1,0,x_2) = \langle\psi^*_{\sigma_1}(0,x_1)\,\psi_{\sigma_1}(0,x_1)\rangle_\lambda \langle\psi^*_{\sigma_2}(0,x_2)\,\psi_{\sigma_2}(0,x_2)\rangle_\lambda + G^{(2)}_{\lambda,\sigma_1\sigma_2}(0,x_1,0,x_2)\,, \tag{3.41}$$

is related to the probability to find one fermion with spin σ_1 at point x_1 and another fermion with spin σ_2 at point x_2.[2] To see this, we compute $Z^{(2)}_{\lambda,\sigma_1\sigma_2}$ in the operator formalism:

$$\begin{aligned} Z^{(2)}_{\lambda,\sigma_1\sigma_2}(0,x_1,0,x_2) &= \langle\Psi_{\mathrm{gs},\lambda}|\hat{n}_\sigma(x_1)\,\hat{n}_{\sigma'}(x_2)|\Psi_{\mathrm{gs},\lambda}\rangle \\ &= n_{\mathrm{gs},\lambda,\sigma_1}(x_1)\,\delta(x_1-x_2)\,\delta_{\sigma_1,\sigma_2} \\ &\quad + N_{\sigma_1}\left(N_{\sigma_2}-\delta_{\sigma_1,\sigma_2}\right)\int_{x_3}\cdots\int_{x_N} |\Psi_{\mathrm{gs},\lambda}(x_1,\sigma_1,x_2,\sigma_2,\ldots,x_N,\sigma_N)|^2\,, \end{aligned} \tag{3.42}$$

From these expressions and Eq. (3.41), we read off the following exact identities for the density-density correlation functions $Z^{(2)}_{\lambda,\sigma_1\sigma_2}$ and $G^{(2)}_{\lambda,\sigma_1\sigma_2}$, respectively:

$$\int_{x_1}\int_{x_2} Z^{(2)}_{\lambda,\sigma_1\sigma_2}(0,x_1,0,x_2) = N_{\sigma_1}N_{\sigma_2} \quad \text{and} \quad \int_{x_1}\int_{x_2} G^{(2)}_{\lambda,\sigma_1\sigma_2}(0,x_1,0,x_2) = 0\,. \tag{3.43}$$

Moreover, we find

$$\sum_{\sigma_1\sigma_2}\int_{x_1}\int_{x_2} Z^{(2)}_{\lambda,\sigma_1\sigma_2}(0,x_1,0,x_2) = N^2 \quad \text{and} \quad \sum_{\sigma_1\sigma_2}\int_{x_1}\int_{x_2} G^{(2)}_{\lambda,\sigma_1\sigma_2}(0,x_1,0,x_2) = 0\,. \tag{3.44}$$

[2] We have set $\tau_1 = \tau_2 = 0$ again without loss of generality.

For convenience, we now define

$$\Phi_{N,\lambda,\sigma_1\sigma_2}(x_1,x_2) = \int_{x_3}\cdots\int_{x_N} |\Psi_{\mathrm{gs},\lambda}(x_1,\sigma_1,x_2,\sigma_2,x_3,\sigma_3,\ldots,x_N,\sigma_N)|^2\,, \tag{3.45}$$

which describes the probability to find a fermion with spin σ_1 at position x_1 and simultaneously a fermion with spin σ_2 at position x_2, up to a suitable normalization. Apparently, the spin-σ ground-state density and the quantity $\Phi_{N,\lambda,\sigma,\sigma_2}(x,x_2)$ are closely related:

$$n_{\mathrm{gs},\lambda,\sigma}(x) = N_\sigma \int_{x_2} \Phi_{N,\lambda,\sigma\sigma_2}(x,x_2)\,. \tag{3.46}$$

Neglecting fluctuation effects and assuming that the positions x_1 and x_2 are far away from each other, we obtain

$$\Phi_{N,\lambda,\sigma_1\sigma_2}(x_1,x_2) \simeq \frac{1}{N_{\sigma_1}(N_{\sigma_2}-\delta_{\sigma_1,\sigma_2})} n_{\mathrm{gs},\lambda,\sigma_1}(x_1)\, n_{\mathrm{gs},\lambda,\sigma_2}(x_2)\,. \tag{3.47}$$

Moreover, we deduce the following exact relation from Eq. (3.42):

$$\begin{aligned}&\Phi_{N,\lambda,\sigma_1\sigma_2}(x_1,x_2) = \\ &\quad\frac{1}{N_{\sigma_1}(N_{\sigma_2}-\delta_{\sigma_1,\sigma_2})}\left(n_{\mathrm{gs},\lambda,\sigma_1}(x_1)\, n_{\mathrm{gs},\lambda,\sigma_2}(x_2) + G^{(2)}_{\lambda,\sigma_1\sigma_2}(0,x_1,0,x_2) - n_{\mathrm{gs},\lambda,\sigma_1}(x_1)\,\delta(x_1-x_2)\,\delta_{\sigma_1,\sigma_2}\right).\end{aligned} \tag{3.48}$$

Due to *Pauli* blocking, we have $\Phi_{N,\lambda,\sigma\sigma}(x,x) = 0$. For $x_1 \to x_2$, we therefore find

$$Z^{(2)}_{\lambda,\sigma\sigma}(0,x_1,0,x_2) = G^{(2)}_{\lambda,\sigma\sigma}(0,x_1,0,x_2) + n_{\mathrm{gs},\lambda,\sigma}(x_1)\, n_{\mathrm{gs},\lambda,\sigma}(x_2) \overset{x_1\to x_2}{\sim} n_{\mathrm{gs},\lambda,\sigma}(x_1)\delta(x_1-x_2)\,, \tag{3.49}$$

which also follows directly from an evaluation of Eq. (3.28).

Now we want to have a closer look at the case $N = 2$. From Eq. (3.48) we obtain the absolute square of the two-body wavefunction:

$$\begin{aligned}&|\Psi_{\mathrm{gs},\lambda}(x_1,\sigma_1,x_2,\sigma_2)|^2 \\ &\quad= \frac{1}{1+\delta_{\sigma_1,\sigma_2}}\left(n_{\mathrm{gs},\lambda,\sigma_1}(x_1)\, n_{\mathrm{gs},\lambda,\sigma_2}(x_2) + G^{(2)}_{\lambda,\sigma_1\sigma_2}(0,x_1,0,x_2) - n_{\mathrm{gs},\lambda,\sigma_1}(x_1)\,\delta(x_1-x_2)\,\delta_{\sigma_1,\sigma_2}\right),\end{aligned} \tag{3.50}$$

which gives the probability density to find one fermion with spin σ_1 at point x_1 and the other fermion with spin σ_2 at point x_2.

Specifically for the case of two identical fermions, where the two particles have the same spin, we obtain

$$|\Psi_{\mathrm{gs},\lambda}(x_1,x_2)|^2 = \frac{1}{2}\left(n_{\mathrm{gs},\lambda}(x_1) n_{\mathrm{gs},\lambda}(x_2) + G^{(2)}_{\lambda}(0,x_1,0,x_2) - n_{\mathrm{gs},\lambda}(x_1)\delta(x_1-x_2)\right), \tag{3.51}$$

where we dropped the spin indices, because all spin-sums would only sum over one possible state.

In the case of two different spin species, where $N_\uparrow = N_\downarrow = 1$ and the system contains one spin-up and one spin-down fermion, the absolute square of the wavefunction can be obtained by

$$|\Psi_{\mathrm{gs},\lambda,\uparrow\downarrow}(x_1,x_2)|^2 = n_{\mathrm{gs},\lambda,\uparrow}(x_1)\, n_{\mathrm{gs},\lambda,\downarrow}(x_2) + G^{(2)}_{\lambda,\uparrow\downarrow}(0,x_1,0,x_2)\,. \tag{3.52}$$

This implies that one can compute the absolute square of the wavefunction for $N = 2$, i. e. the probability density to find one fermion at point x_1 and the other one at point x_2, directly from the density $n_{\mathrm{gs},\lambda}$ and the density-density correlation function $G^{(2)}_{\lambda,\sigma_1\sigma_2}$ as, e. g., computed with our DFT-RG approach. To extract the absolute square of the

wavefunction associated with the relative motion $|\varphi_{N,\lambda}|^2$, i. e. the so-called intrinsic density, it is convenient to introduce new coordinates. For $N=2$, we use $R=\frac{1}{2}(x_1+x_2)$ and $r=x_1-x_2$. The intrinsic density for the two fermion system is then given by

$$|\varphi_{N=2,\lambda,\sigma\sigma'}(r)|^2 = 2\int_{-\frac{L-|r|}{2}}^{\frac{L-|r|}{2}} \mathrm{d}R\, |\Psi_{\mathrm{gs},\lambda,\sigma\sigma'}(R+\tfrac{1}{2}|r|, R-\tfrac{1}{2}|r|)|^2, \tag{3.53}$$

where we have used the symmetry under $r\to -r$ to define r such that $0\le r\le L$. This equation can be used to obtain the intrinsic density for the system of two identical fermions as well as for the system with one spin-up and one spin-down fermion. Although Γ_λ is not a functional of the intrinsic density but only of ρ, we can obtain the intrinsic density from the correlation functions $\Gamma_\lambda^{(n)}$ determining uniquely the density functional Γ_λ. We stress that the density $\rho_{\mathrm{gs},\lambda}$ minimizing Γ_λ should by no means be confused with the intrinsic density. In fact, for a given N-body system (with $N>1$), the intrinsic density cannot be extracted from $\rho_{\mathrm{gs},\lambda}$.

For $N\ge 3$, it is possible to extract $|\Psi_{\mathrm{gs},\lambda}(x_1,\sigma_1,\ldots,x_N,\sigma_N)|^2$ from the N-density correlation function $G^{(N)}_{\lambda,\sigma_1\ldots\sigma_N}$. The associated intrinsic density is then obtained along the lines of the case $N=2$ by, e. g., using *Jacobi* coordinates. We add that the computation of the $G^{(N)}_{\lambda,\sigma_1\ldots\sigma_N}$ functions and therefore of $|\Psi_{\mathrm{gs},\lambda}(x_1,\sigma_1,\ldots,x_N,\sigma_N)|^2$ in general requires the fully time-dependent density correlation functions $G^{(m)}_{\lambda,\sigma_1\ldots\sigma_m}(\tau_1,x_1,\ldots,\tau_m,x_m)$ with $1\le m\le N+2$, as we shall see below.

We now show that excited states can be extracted from the time-dependent density-density correlation function $G^{(2)}_\lambda$. To this end, we first consider the spectral decomposition of $Z^{(2)}_{\lambda,\sigma_1\sigma_2}$ within the operator formalism,

$$Z^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1,x_1,\tau_2,x_2) = \sum_{n=0}^{\infty}\langle\Psi_{\mathrm{gs},\lambda}|\hat\psi^\dagger_{\sigma_1}(x_1)\,\hat\psi_{\sigma_1}(x_1)|\Psi^{(n)}_\lambda\rangle\langle\Psi^{(n)}_\lambda|\hat\psi^\dagger_{\sigma_2}(x_2)\,\hat\psi_{\sigma_2}(x_2)|\Psi_{\mathrm{gs},\lambda}\rangle\,\mathrm{e}^{-(E_{n,\lambda}-E_{0,\lambda})|\tau_1-\tau_2|}, \tag{3.54}$$

which is obtained by inserting a suitably chosen $\mathbb{1}$-operator,

$$\mathbb{1} = \sum_{n=0}^{\infty}|\Psi^{(n)}_\lambda\rangle\langle\Psi^{(n)}_\lambda|, \tag{3.55}$$

into the analogue of Eq. (3.26) in the *Heisenberg* picture. Here, $|\Psi^{(n)}_\lambda\rangle$ are the eigenstates of the N-body problem with energies $E_{n,\lambda}$, ordered such that $E_\lambda\equiv E_{0,\lambda}<E_{1,\lambda}<\ldots$ and $|\Psi_{\mathrm{gs},\lambda}\rangle\equiv|\Psi^{(0)}_\lambda\rangle$.[3] From the relation (3.28) between $Z^{(2)}_{\lambda,\sigma_1\sigma_2}$ and $G^{(2)}_{\lambda,\sigma_1\sigma_2}$, it then follows that

$$G^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1,x_1,\tau_2,x_2) = \sum_{n=1}^{\infty}\langle\Psi_{\mathrm{gs},\lambda}|\hat\psi^\dagger_{\sigma_1}(x_1)\,\hat\psi_{\sigma_1}(x_1)|\Psi^{(n)}_\lambda\rangle\langle\Psi^{(n)}_\lambda|\hat\psi^\dagger_{\sigma_2}(x_2)\,\hat\psi_{\sigma_2}(x_2)|\Psi_{\mathrm{gs},\lambda}\rangle\,\mathrm{e}^{-(E_{n,\lambda}-E_{0,\lambda})|\tau_1-\tau_2|}. \tag{3.56}$$

From this expression, we deduce that the first excited state can be extracted directly from $G^{(2)}_{\lambda,\sigma_1\sigma_2}$ in the limit of large time differences:

$$(E_{1,\lambda}-E_{0,\lambda}) = -\lim_{|\tau|\to\infty}\frac{1}{|\tau|}\ln G^{(2)}_{\lambda,\sigma\sigma}(\tau,0,0,0), \tag{3.57}$$

where $E_{0,\lambda}$ is the ground-state energy and we have set $\tau_2=0$ and $\tau_1=\tau$ without loss of generality. In addition, we have set $x_1=x_2=0$ to ensure that the first excited state is included in the sum (3.56). In fact, we can write

$$\hat\psi^\dagger_\sigma(x)\,\hat\psi_\sigma(x) = \sum_{k,l}\hat a^\dagger_{\sigma,k}\hat a_{\sigma,l}\,\phi^*_{\sigma,k}(x)\,\phi_{\sigma,l}(x), \tag{3.58}$$

[3] Here, we assume that the ground state is not degenerate.

where $\hat{a}_k^\dagger$ creates and $\hat{a}_l$ annihilates a fermion with spin σ and momenta p_k and p_l, respectively. The position-space representations of the one-particle eigenstates satisfy the following conditions:

$$\int_x \phi^*_{\sigma,m}(x)\,\phi_{\sigma,n}(x) = \delta_{m,n} \quad \text{and} \quad \sum_n \phi^*_{\sigma,n}(x_1)\,\phi_{\sigma,n}(x_2) = \delta(x_1 - x_2)\,, \tag{3.59}$$

where $n, m \in \mathbb{Z}$.[4]

From Eq. (3.58), we conclude that it is possible to choose x_1 and x_2 in Eq. (3.56) such that, at least in the non-interacting limit, the matrix element $\langle \Psi_{\mathrm{gs},\lambda} | \hat{\psi}^\dagger_\sigma(x_i)\,\hat{\psi}_\sigma(x_i) | \Psi^{(n)}_\lambda \rangle$ vanishes for specific excited states, depending on the momentum difference of the created and annihilated fermion.

From Eqs. (3.56) and (3.58), we also obtain the generalizations of the relations in Eq. (3.43) and Eq. (3.44) for time-dependent density-density correlation functions using $\hat{N}_\sigma |\Psi\rangle = N_\sigma |\Psi\rangle$:

$$\int_{x_1}\int_{x_2} Z^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1, x_1, \tau_2, x_2) = N_{\sigma_1} N_{\sigma_2} \quad \text{and} \quad \int_{x_i} G^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1, x_1, \tau_2, x_2) = 0\,, \tag{3.60}$$

$$\sum_{\sigma_1,\sigma_2}\int_{x_1}\int_{x_2} Z^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1, x_1, \tau_2, x_2) = N^2 \quad \text{and} \quad \sum_{\sigma_1,\sigma_2}\int_{x_i} G^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1, x_1, \tau_2, x_2) = 0\,, \tag{3.61}$$

where $i \in \{1, 2\}$. These relations can be further generalized to the case of n-density correlation functions. Using Eq. (3.58) and the spectral decomposition of the n-density correlation function, it follows that

$$\int_{x_1}\cdots\int_{x_n} Z^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}(\chi_1, \ldots, \chi_n) = N_{\sigma_1}\cdots N_{\sigma_n} \quad \text{and} \quad \int_{x_i} G^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}(\chi_1, \ldots, \chi_n) = 0\,, \tag{3.62}$$

$$\sum_{\sigma_1,\ldots,\sigma_n}\int_{x_1}\cdots\int_{x_n} Z^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}(\chi_1, \ldots, \chi_n) = N^n \quad \text{and} \quad \sum_{\sigma_1,\ldots,\sigma_n}\int_{x_i} G^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}(\chi_1, \ldots, \chi_n) = 0\,, \tag{3.63}$$

where $i \in \{1, \ldots, n\}$. As we shall see below, these exact relations are useful to analyze the DFT-RG flows on very general grounds.

In addition to the energy of the first excited state, it is possible to extract a so-called spectral function $\Omega_{\lambda,\sigma_1\sigma_2}$ from the density-density correlation function which gives access to the energies of higher excited states as well. To see this, we consider the Fourier transformation of $G^{(2)}_{\lambda,\sigma_1\sigma_2}$ with respect to the imaginary time τ :

$$\tilde{G}^{(2)}_{\lambda,\sigma_1\sigma_2}(\omega, x_1, x_2) = \int_{-\infty}^{\infty} \frac{\mathrm{d}E}{2\pi} \frac{2E}{\omega^2 + E^2}\, \Omega_{\lambda,\sigma_1\sigma_2}(E, x_1, x_2)\,, \tag{3.64}$$

where

$$G^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1, x_1, \tau_2, x_2) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}\, \tilde{G}^{(2)}_{\lambda,\sigma_1\sigma_2}(\omega, x_1, x_2)\, \mathrm{e}^{-\mathrm{i}\omega(\tau_1 - \tau_2)} \tag{3.65}$$

and the spectral function Ω_λ is defined as

$$\Omega_{\lambda,\sigma_1\sigma_2}(E, x_1, x_2) = 2\pi \sum_{n=1}^{\infty} \langle \Psi_{\mathrm{gs},\lambda} | \hat{\psi}^\dagger_{\sigma_1}(x_1)\,\hat{\psi}_{\sigma_1}(x_1) | \Psi^{(n)}_\lambda \rangle \langle \Psi^{(n)}_\lambda | \hat{\psi}^\dagger_{\sigma_2}(x_2)\,\hat{\psi}_{\sigma_2}(x_2) | \Psi_{\mathrm{gs},\lambda} \rangle\, \delta(E - (E_{n,\lambda} - E_{0,\lambda}))\,. \tag{3.66}$$

Within our DFT-RG approach, we have direct access to the density-density correlation function $G^{(2)}_{\lambda,\sigma_1\sigma_2}$. To obtain the spectral function, we therefore need to solve Eq. (3.64) for $\Omega_{\lambda,\sigma_1\sigma_2}$. Using

$$\frac{2E}{\omega^2 + E^2} = \frac{1}{-\mathrm{i}\omega + E} - \frac{1}{-\mathrm{i}\omega - E} \quad \text{and} \quad \lim_{\eta\to 0^+} \frac{1}{\omega \pm \mathrm{i}\eta} = \mathrm{P}\frac{1}{\omega} \mp \mathrm{i}\pi\delta(\omega)\,, \tag{3.67}$$

[4] In this thesis we will use plane waves as basis functions. In general, one can choose a suitable basis for the problem under consideration. For fermions in a harmonic trap one could for example consider harmonic oscillator eigenfunctions as basis functions.

where P is the principal value, we find that Eq. (3.64) can indeed be solved for $\Omega_{\lambda,\sigma_1\sigma_2}$:

$$\Omega_{\lambda,\sigma_1\sigma_2}(E,x_1,x_2) = 2\lim_{\eta\to 0^+} \operatorname{Im} \tilde{G}^{(2)}_{\lambda,\sigma_1\sigma_2}(\mathrm{i}E-\eta,x_1,x_2)\,. \tag{3.68}$$

Moreover, we observe that $\Omega_{\lambda,\sigma_1\sigma_2}$ obeys the following "sum rule":

$$\int_{-\infty}^{\infty} \frac{\mathrm{d}E}{2\pi} \Omega_{\lambda,\sigma_1\sigma_2}(E,x,y) = G^{(2)}_{\lambda,\sigma_1\sigma_2}(0,x,0,y)\,. \tag{3.69}$$

Thus, the spectral function is obtained from an analytic continuation of the Fourier transform of the density-density correlation function, in complete analogy to the case of 1PI correlation functions, see, e. g., Refs. [62, 63]. If an analytic solution of the flow equation for the density-density correlation function is not available, the analytic continuation has to be performed numerically which is in general expected to be a highly non-trivial problem. However, since $\tilde{G}^{(2)}$ is invariant under $\omega \to -\omega$ and $\tilde{G}^{(2)}_{\lambda,\sigma_1\sigma_2} \sim 1/\omega^2$ in the large ω-limit, the computation of Ω_λ may in principle be achieved by fitting the numerical results for $\tilde{G}^{(2)}_{\lambda,\sigma_1\sigma_2}$ to Padé approximants respecting these constraints. From the analytic continuation of the Padé approximants, the spectral function can then be obtained. In any case, we shall focus on the computation of ground-state properties in our numerical studies presented below and defer the computation of excited states within our DFT-RG formalism to future work.

3.3 Flow Equations for the Density Correlation Functions

We will now derive the flow equations for the energy, density and the density-correlation functions. We assume here and in the following that the interaction potential is symmetrical regarding interchanges of the indice pairs $(\sigma_1,x_1) \leftrightarrow (\sigma_2,x_2)$:

$$U_{\sigma_1\sigma_2}(x_1,x_2) = U_{\sigma_2\sigma_1}(x_2,x_1)\,. \tag{3.70}$$

Since the ground-state energy is essentially proportional to $W_\lambda[0]$, see Eq. (2.55), it suffices to consider the flow equation for the latter which is obtained by setting $J_\sigma = 0$ in Eq. (3.34):

$$\begin{aligned}\partial_\lambda W_\lambda[0] = &-\frac{1}{2}\sum_{\sigma_1\sigma_2}\int_{\tau_1}\int_{x_1}\int_{x_2} n_{\mathrm{gs},\lambda,\sigma_1}(x_1)\,U_{\sigma_1\sigma_2}(x_1,x_2)\,n_{\mathrm{gs},\lambda,\sigma_2}(x_2)\\ &-\frac{1}{2}\sum_{\sigma_1\sigma_2}\int_{\tau_1}\int_{x_1}\int_{x_2} U_{\sigma_1\sigma_2}(x_1,x_2)\Big(G^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1,x_1,\tau_1,x_2) - n_{\mathrm{gs},\lambda,\sigma_2}(x_2)\,\delta_{\sigma_2,\sigma_1}\,\delta(x_2-x_1)\Big)\,.\end{aligned} \tag{3.71}$$

The flow equation for the density $n_{\mathrm{gs},\lambda,\sigma}$ is obtained by taking a functional derivative of Eq. (3.34) with respect to the sources $\{J_\sigma\}$ and then setting $J_\sigma = 0$. It reads:

$$\begin{aligned}\partial_\lambda n_{\mathrm{gs},\lambda,\sigma}(x) = &-\sum_{\sigma_1\sigma_2}\int_{\tau_1}\int_{x_1}\int_{x_2} n_{\mathrm{gs},\lambda,\sigma_1}(x_1)\,U_{\sigma_1\sigma_2}(x_1-x_2)\,G^{(2)}_{\lambda,\sigma_2\sigma}(\tau_1,x_2,0,x)\\ &-\frac{1}{2}\sum_{\sigma_1\sigma_2}\int_{\tau_1}\int_{x_1}\int_{x_2} U_{\sigma_1\sigma_2}(x_1-x_2)\Big(G^{(3)}_{\lambda,\sigma_1\sigma_2\sigma}(\tau_1,x_2,\tau_1,x_1,0,x)\\ &\qquad -\delta(x_2-x_1)\,\delta_{\sigma_2,\sigma_1}\,G^{(2)}_{\lambda,\sigma_1\sigma}(\tau_1,x_1,0,x)\Big)\,.\end{aligned} \tag{3.72}$$

This flow equation depends on the density itself, the density-density correlation function $G^{(2)}_{\lambda,\sigma_1\sigma_2}$ and the three-density correlation function $G^{(3)}_{\lambda,\sigma_1\sigma_2\sigma_3}$. From Eqs. (3.62) and (3.63), it follows immediately that

$$\int_x \partial_\lambda n_{\mathrm{gs},\lambda,\sigma}(x) = 0 \qquad \text{and} \qquad \int_x \partial_\lambda n_{\mathrm{gs},\lambda}(x) = 0\,. \tag{3.73}$$

Thus, the fermion number remains constant in the RG flow and is therefore indeed fixed by the initial condition. Also the number of spin-σ fermions is constant in the RG flow.

The flow equation for the density-density correlation function $G^{(2)}_{\lambda}$ can be derived by taking the second functional derivative of Eq. (3.34) with respect to the sources $\{J_\sigma\}$ and then setting $J_\sigma = 0$. We find:

$$\begin{aligned}\partial_\lambda G^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1,x_1,\tau_2,x_2) = &-\sum_{\sigma_3\sigma_4}\int_{\tau_3}\int_{x_3}\int_{x_4} G^{(2)}_{\lambda,\sigma_1\sigma_3}(\tau_1,x_1,\tau_3,x_3)\,U_{\sigma_3\sigma_4}(x_3-x_4)\,G^{(2)}_{\lambda,\sigma_4\sigma_2}(\tau_3,x_4,\tau_2,x_2)\\ &-\sum_{\sigma_3\sigma_4}\int_{\tau_3}\int_{x_3}\int_{x_4} n_{\mathrm{gs},\lambda,\sigma_3}(x_3)\,U_{\sigma_3\sigma_4}(x_3-x_4)\,G^{(3)}_{\lambda,\sigma_4\sigma_1\sigma_2}(\tau_3,x_4,\tau_1,x_1,\tau_2,x_2)\\ &-\frac{1}{2}\sum_{\sigma_3\sigma_4}\int_{\tau_3}\int_{x_3}\int_{x_4} U_{\sigma_3\sigma_4}(x_3-x_4)\Big(G^{(4)}_{\lambda,\sigma_4\sigma_3\sigma_1\sigma_2}(\tau_3,x_4,\tau_3,x_3,\tau_1,x_1,\tau_2,x_2)\\ &-\delta(x_4-x_3)\,\delta_{\sigma_4,\sigma_3}\,G^{(3)}_{\lambda,\sigma_3\sigma_1\sigma_2}(\tau_3,x_3,\tau_1,x_1,\tau_2,x_2)\Big). \quad (3.74)\end{aligned}$$

The flow equation for $G^{(2)}_{\lambda,\sigma_1\sigma_2}$ depends on the density, the density-density correlation function $G^{(2)}_{\lambda,\sigma_1\sigma_2}$, the three-density correlation function $G^{(3)}_{\lambda,\sigma_1\sigma_2\sigma_3}$ and the four-density correlation function $G^{(4)}_{\lambda,\sigma_1\ldots\sigma_4}$. Using Eqs. (3.62) and (3.63) again, we can look at the equation from a more general point of view and observe

$$\int_{x_1}\int_{x_2}\partial_\lambda G^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1,x_1,\tau_2,x_2)=0 \qquad \text{and} \qquad \sum_{\sigma_1\sigma_2}\int_{x_1}\int_{x_2}\partial_\lambda G^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1,x_1,\tau_2,x_2)=0\,. \quad (3.75)$$

Loosely speaking, this implies that the normalization of the ground-state wavefunction is preserved in the RG flow which is necessary to assign a physical interpretation to this correlation function, see also our discussion in Sec. 3.2.

In general the flow equation for the n-density correlation functions can be derived by taking the nth functional derivative of Eq. (3.34) with respect to the sources $\{J_\sigma\}$ and then setting $J_\sigma = 0$.

We show the flow equations up to the flow equation for the four-density correlation function here because we will use the latter to calculate the energy up to fourth order in the perturbative expansion for systems of spin-$1/2$ fermions and a perturbation theory motivated truncation for the DFT-RG formalism in Chap. 7. For the flow equation for the three-density correlation function $G^{(3)}_{\lambda,\sigma_1\sigma_2\sigma_3}$ we find

$$\begin{aligned}&\partial_\lambda G^{(3)}_{\lambda,\sigma_1\sigma_2\sigma_3}(\tau_1,x_1,\tau_2,x_2,\tau_3,x_3)\\ &\quad=-\sum_{\sigma_4\sigma_5}\int_{\tau_4}\int_{x_4}\int_{x_5}\Big(G^{(2)}_{\lambda,\sigma_1\sigma_4}(\tau_1,x_1,\tau_4,x_4)\,U_{\sigma_4\sigma_5}(x_4-x_5)\,G^{(3)}_{\lambda,\sigma_5\sigma_2\sigma_3}(\tau_4,x_5,\tau_2,x_2,\tau_3,x_3)\\ &\qquad\qquad+G^{(2)}_{\lambda,\sigma_2\sigma_4}(\tau_2,x_2,\tau_4,x_4)\,U_{\sigma_4\sigma_5}(x_4-x_5)\,G^{(3)}_{\lambda,\sigma_5\sigma_1\sigma_3}(\tau_4,x_5,\tau_1,x_1,\tau_3,x_3)\\ &\qquad\qquad+G^{(2)}_{\lambda,\sigma_3\sigma_4}(\tau_3,x_3,\tau_4,x_4)\,U_{\sigma_4\sigma_5}(x_4-x_5)\,G^{(3)}_{\lambda,\sigma_5\sigma_1\sigma_2}(\tau_4,x_5,\tau_1,x_1,\tau_2,x_2)\Big)\\ &\qquad-\sum_{\sigma_4\sigma_5}\int_{\tau_4}\int_{x_4}\int_{x_5} n_{\mathrm{gs},\lambda,\sigma_4}(x_4)\,U_{\sigma_4\sigma_5}(x_4-x_5)\,G^{(4)}_{\lambda,\sigma_5\sigma_1\sigma_2\sigma_3}(\tau_4,x_5,\tau_1,x_1,\tau_2,x_2,\tau_3,x_3)\\ &\qquad-\frac{1}{2}\sum_{\sigma_4\sigma_5}\int_{\tau_4}\int_{x_4}\int_{x_5} U_{\sigma_4\sigma_5}(x_4-x_5)\Big(G^{(5)}_{\lambda,\sigma_5\sigma_4\sigma_1\sigma_2\sigma_3}(\tau_4,x_5,\tau_4,x_4,\tau_1,x_1,\tau_2,x_2,\tau_3,x_3)\\ &\qquad\qquad-\delta(x_5-x_4)\,\delta_{\sigma_5,\sigma_4}\,G^{(4)}_{\lambda,\sigma_4\sigma_1\sigma_2\sigma_3}(\tau_4,x_4,\tau_1,x_1,\tau_2,x_2,\tau_3,x_3)\Big) \quad (3.76)\end{aligned}$$

and for the flow equation for the four-density correlation function $G^{(4)}_{\lambda,\sigma_1\ldots\sigma_4}$ we find:

$$
\begin{aligned}
&\partial_\lambda G^{(4)}_{\lambda,\sigma_1\sigma_2\sigma_3\sigma_4}(\tau_1,x_1,\tau_2,x_2,\tau_3,x_3,\tau_4,x_4)\\
&\quad=-\sum_{\sigma_5\sigma_6}\int_{\tau_5}\int_{x_5}\int_{x_6}\Big(G^{(3)}_{\lambda,\sigma_1\sigma_2\sigma_5}(\tau_1,x_1,\tau_2,x_2,\tau_5,x_5)\,U_{\sigma_5\sigma_6}(x_5-x_6)\,G^{(3)}_{\lambda,\sigma_6\sigma_3\sigma_4}(\tau_5,x_6,\tau_3,x_3,\tau_4,x_4)\\
&\qquad\qquad+G^{(3)}_{\lambda,\sigma_1\sigma_3\sigma_5}(\tau_1,x_1,\tau_3,x_3,\tau_5,x_5)\,U_{\sigma_5\sigma_6}(x_5-x_6)\,G^{(3)}_{\lambda,\sigma_6\sigma_2\sigma_4}(\tau_5,x_6,\tau_2,x_2,\tau_4,x_4)\\
&\qquad\qquad+G^{(3)}_{\lambda,\sigma_1\sigma_4\sigma_5}(\tau_1,x_1,\tau_4,x_4,\tau_5,x_5)\,U_{\sigma_5\sigma_6}(x_5-x_6)\,G^{(3)}_{\lambda,\sigma_6\sigma_2\sigma_3}(\tau_5,x_6,\tau_2,x_2,\tau_3,x_3)\Big)\\
&\quad-\sum_{\sigma_5\sigma_6}\int_{\tau_5}\int_{x_5}\int_{x_6}\Big(G^{(2)}_{\lambda,\sigma_1\sigma_5}(\tau_1,x_1,\tau_5,x_5)\,U_{\sigma_5\sigma_6}(x_5-x_6)\,G^{(4)}_{\lambda,\sigma_6\sigma_2\sigma_3\sigma_4}(\tau_5,x_6,\tau_2,x_2,\tau_3,x_3,\tau_4,x_4)\\
&\qquad\qquad+G^{(2)}_{\lambda,\sigma_2\sigma_5}(\tau_2,x_2,\tau_5,x_5)\,U_{\sigma_5\sigma_6}(x_5-x_6)\,G^{(4)}_{\lambda,\sigma_6\sigma_1\sigma_3\sigma_4}(\tau_5,x_6,\tau_1,x_1,\tau_3,x_3,\tau_4,x_4)\\
&\qquad\qquad+G^{(2)}_{\lambda,\sigma_3\sigma_5}(\tau_3,x_3,\tau_5,x_5)\,U_{\sigma_5\sigma_6}(x_5-x_6)\,G^{(4)}_{\lambda,\sigma_6\sigma_1\sigma_2\sigma_4}(\tau_5,x_6,\tau_1,x_1,\tau_2,x_2,\tau_4,x_4)\\
&\qquad\qquad+G^{(2)}_{\lambda,\sigma_4\sigma_5}(\tau_4,x_4,\tau_5,x_5)\,U_{\sigma_5\sigma_6}(x_5-x_6)\,G^{(4)}_{\lambda,\sigma_6\sigma_1\sigma_2\sigma_3}(\tau_5,x_6,\tau_1,x_1,\tau_2,x_2,\tau_3,x_3)\Big)\\
&\quad-\sum_{\sigma_5\sigma_6}\int_{\tau_5}\int_{x_5}\int_{x_6}n_{gs,\lambda,\sigma_5}(x_5)\,U_{\sigma_5\sigma_6}(x_5-x_6)\,G^{(5)}_{\lambda,\sigma_6\sigma_1\sigma_2\sigma_3\sigma_4}(\tau_5,x_6,\tau_1,x_1,\tau_2,x_2,\tau_3,x_3,\tau_4,x_4)\\
&\quad-\frac{1}{2}\sum_{\sigma_5\sigma_6}\int_{\tau_5}\int_{x_5}\int_{x_6}U_{\sigma_5\sigma_6}(x_5-x_6)\Big(G^{(6)}_{\lambda,\sigma_6\sigma_5\sigma_1\sigma_2\sigma_3\sigma_4}(\tau_5,x_6,\tau_5,x_5,\tau_1,x_1,\tau_2,x_2,\tau_3,x_3,\tau_4,x_4)\\
&\qquad\qquad-\delta(x_6-x_5)\,\delta_{\sigma_6,\sigma_5}\,G^{(5)}_{\lambda,\sigma_5\sigma_1\sigma_2\sigma_3\sigma_4}(\tau_5,x_5,\tau_1,x_1,\tau_2,x_2,\tau_3,x_3,\tau_4,x_4)\Big)\,. \qquad (3.77)
\end{aligned}
$$

In general, the flow of the n-density correlation function $G^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}(\tau_1,x_1,\ldots,\tau_n,x_n)$ depends on the density correlation functions $G^{(m)}_{\lambda,\sigma_1\ldots\sigma_m}(\tau_1,x_1,\ldots,\tau_m,x_m)$ with $1\le m\le N+2$. Using Eqs. (3.62) and (3.63) it follows in general:

$$
\int_{x_1}\cdots\int_{x_n}\partial_\lambda G^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}(\tau_1,x_1,\ldots,\tau_n,x_n)=0\quad\text{and}\quad\sum_{\sigma_1,\ldots,\sigma_n}\int_{x_1}\ldots\int_{x_n}\partial_\lambda G^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}(\tau_1,x_1,\ldots,\tau_n,x_n)=0\,. \qquad (3.78)
$$

3.4 Many-Body Perturbation Theory

We now show that our DFT-RG approach allows us to recover the perturbative expansion in a systematic fashion. Let us consider a general two-body interaction to discuss the connection of our approach to many-body perturbation theory, i. e. an expansion of observables, such as the ground-state energy, in powers of some (small) dimensionless parameter $\bar{g}$. For convenience, we shall assume in the following that the two-body interaction U can be written as a product of a coupling parameter g with dimension of inverse length and a generally space-dependent shape function $\mathfrak{U}$ with dimension of inverse length as

$$
U_{\sigma_1\sigma_2}(x_1-x_2)=g\,\mathfrak{U}_{\sigma_1\sigma_2}(x_1-x_2)\,. \qquad (3.79)
$$

In particular, we shall assume that the coupling is independent of the spin. To define a dimensionless coupling parameter $\bar{g}$ we need a suitable quantity with dimension of inverse length. For homogeneous systems, like fermions in a box with (anti)periodic boundary conditions, we can use the homogeneous density to render the coupling constant dimensionless. This will be the case in our model studies, see Chaps. 6 and 7. For fermions in a harmonic trap, for example, we may use the density of the non-interacting system in the center of the trap or the oscillator length $\sim 1/\sqrt{\omega}$ to render g dimensionless. The perturbative expansion of the ground-state energy can now be defined as follows:

$$
E_\lambda=N\left(E^{(0)}+E^{(1)}_\lambda\,\bar{g}+\frac{1}{2}E^{(2)}_\lambda\,\bar{g}^2+\ldots\right), \qquad (3.80)
$$

where $E_\lambda^{(i)}$ is associated with the energy correction of order $\mathcal{O}(\bar{g}^i)$ and $E^{(0)} \equiv E_{\lambda=0}/N$ is the ground-state energy of the non-interacting system. In the same way we can expand other quantities, such as the ground-state density and the density-density correlation function. We define:

$$n_{\mathrm{gs},\lambda,\sigma}(x) = n^{(0)}_{\mathrm{gs},\sigma}(x) + n^{(1)}_{\mathrm{gs},\lambda,\sigma}(x)\,\bar{g} + \frac{1}{2} n^{(2)}_{\mathrm{gs},\lambda,\sigma}(x)\,\bar{g}^2 + \dots\,, \tag{3.81}$$

where $n^{(0)}_{\mathrm{gs},\sigma} \equiv n_{\mathrm{gs},\lambda=0,\sigma}$ is the ground-state density of the spin-σ fermions of the non-interacting system, and

$$G^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1,x_1,\tau_2,x_2) = G^{(2,0)}_{\sigma_1\sigma_2}(\tau_1,x_1,\tau_2,x_2) + G^{(2,1)}_{\lambda,\sigma_1\sigma_2}(\tau_1,x_1,\tau_2,x_2)\,\bar{g} + \frac{1}{2} G^{(2,2)}_{\lambda,\sigma_1\sigma_2}(\tau_1,x_1,\tau_2,x_2)\,\bar{g}^2 + \dots\,, \tag{3.82}$$

where $G^{(2,0)}_{\sigma_1\sigma_2} \equiv G^{(2)}_{\lambda=0,\sigma_1\sigma_2}$ is the non-interacting density-density correlation function. Density correlation functions of higher order can be expanded accordingly. Thus, the initial conditions for the RG equations for the energy, density and the density correlation functions are simply given by the zeroth order of their perturbative expansions.

Using Eq. (3.14) we obtain the flow equation for the energy from Eq. (3.71):

$$\begin{aligned}\partial_\lambda E_\lambda =& \frac{1}{2}\sum_{\sigma_1\sigma_2}\int_{x_1}\int_{x_2} n_{\mathrm{gs},\lambda,\sigma_1}(x_1)\,U_{\sigma_1\sigma_2}(x_1-x_2)\,n_{\mathrm{gs},\lambda,\sigma_2}(x_2) \\ &+ \frac{1}{2}\sum_{\sigma_1\sigma_2}\int_{x_1}\int_{x_2} U_{\sigma_1\sigma_2}(x_1-x_2)\left(G^{(2)}_{\lambda,\sigma_2\sigma_1}(0,x_2,0,x_1) - n_{\mathrm{gs},\lambda,\sigma_2}(x_2)\,\delta_{\sigma_2,\sigma_1}\,\delta(x_2-x_1)\right).\end{aligned} \tag{3.83}$$

To derive perturbative corrections for the ground-state energy within our formalism we plug the expansions (3.80), (3.81), and (3.82) into this equation. We can obtain flow equations for the energy corrections $E_\lambda^{(i)}$ by comparing the left-hand side and the right-hand side order by order in powers of the coupling parameter $\bar{g}$. Since both terms on the right-hand side of Eq. (3.83) dependent explicitly on U the computation of the leading-order correction $E_\lambda^{(1)}$ only requires the density and density-density correlation function in their zeroth-order approximations, i. e. $n^{(0)}_{\mathrm{gs},\sigma}$ and $G^{(2,0)}_{\sigma_1\sigma_2}$, respectively. The computation of the flow for the second-order correction $E_\lambda^{(2)}$ requires the computation of the leading-order correction to the density and the density-density correlation function, i. e. $n^{(1)}_{\mathrm{gs},\lambda}$ and $G^{(2,1)}_{\lambda,\sigma_1\sigma_2}$, respectively. These considerations can be continued successively and we conclude that we need the corrections $n^{(n-1)}_{\mathrm{gs},\lambda,\sigma}$ for the density and $G^{(2,n-1)}_{\lambda,\sigma_1\sigma_2}$ for the density-density correlation function in order to obtain the n-th energy correction $E_\lambda^{(n)}$.

To obtain the first-order perturbative corrections for the density and the density-density correlator we plug the expansions (3.80), (3.81), (3.82) and, if necessary, the expansions of higher-order density correlation functions in the flow equations of the density (3.72) and the density-density correlator (3.74). We can then again compare the resulting equations order by order in the coupling constant $\bar{g}$. Of course this procedure can be expanded to arbitrary orders of density correlation functions. We shall discuss this in more detail within our model studies in Chaps. 6 and 7.

As already mentioned in Sec. 3.2, for $N = 2$ the absolute square of the wavefunction can be calculated from the density-density correlation function. Also for this quantity an expansion in powers of the coupling $\bar{g}$ can be defined:

$$|\Psi_{\mathrm{gs},\lambda}(x_1,x_2)|^2 = |\Psi^{(0)}_{\mathrm{gs}}(x_1,x_2)|^2 + |\Psi^{(1)}_{\mathrm{gs},\lambda}(x_1,x_2)|^2\,\bar{g} + \dots\,, \tag{3.84}$$

where $|\Psi^{(0)}_{\mathrm{gs}}(x_1,x_2)|^2 = |\Psi_{\mathrm{gs},\lambda=0}(x_1,x_2)|^2$.

From Eq. (3.84), the intrinsic density can be computed in leading order by plugging this expansion into Eq. (3.53).

For completeness, we close this subsection by noting that the spectral function $\Omega_{\lambda,\sigma_1\sigma_2}(E,x_1,x_2)$ in leading order in $\bar{g}$ can also be computed from $G^{(2,1)}_{\lambda,\sigma_1\sigma_2}$, see Sec. 3.2, which gives us access to excited states. To be specific, we have

$$\Omega_{\lambda,\sigma_1\sigma_2}(E,x_1,x_2) = \Omega^{(0)}_{\lambda,\sigma_1\sigma_2}(E,x_1,x_2) + \Omega^{(1)}_{\lambda,\sigma_1\sigma_2}(E,x_1,x_2)\,\bar{g} + \dots\,, \tag{3.85}$$

where

$$\Omega^{(n)}_{\lambda,\sigma_1\sigma_2}(E,x_1,x_2) = 2\lim_{\eta\to 0^+} \mathrm{Im}\,\tilde{G}^{(2,n)}_{\lambda,\sigma_1\sigma_2}(\mathrm{i}E-\eta,x_1,x_2) \tag{3.86}$$

with $\tilde{G}^{(2,n)}_{\lambda}$ being the Fourier transformations of $G^{(2,n)}_{\lambda}$.

The direct connection of our approach to many-body perturbation theory is a very useful feature to guide the construction of systematic approximation schemes for our DFT-RG studies. To reiterate, this does *not* imply that this approach is only perturbative. On the contrary, the solution for, e. g., the density-density correlation function from the flow equation (3.74) includes arbitrarily high orders in the dimensionless parameter $\bar{g}$.

3.5 Hartree Approximation

The so-called *Hartree* approximation can be obtained from the general flow equation (3.35) by dropping the second term on the right-hand side. The latter includes, e. g., the so-called *Fock* term. Dropping the second term on the right-hand side of Eq. (3.35), we can solve the flow equation for $\Gamma_\lambda[\rho]$ analytically. We find

$$\Gamma_\lambda[\{\rho_\sigma\}] = \Gamma_{\lambda=0}[\{\rho_\sigma\}] + \frac{\lambda}{2}\sum_{\sigma_1\sigma_2}\int_{\chi_1}\int_{\chi_2}\rho_{\sigma_1}(\chi_1)\,U_{2\mathrm{b},\sigma_1\sigma_2}(\chi_1,\chi_2)\,\rho_{\sigma_2}(\chi_2)\,, \tag{3.87}$$

where $\Gamma_{\lambda=0}[\{\rho_\sigma\}]$ is simply the 2PPI effective action of the non-interacting (initial) system at $\lambda = 0$. From the definition of the ground state,

$$\left.\frac{\delta\Gamma_\lambda[\{\rho_\sigma\}]}{\delta\rho_\sigma}\right|_{\rho_\sigma=\rho_{\mathrm{gs},\lambda,\sigma}} = 0\,, \tag{3.88}$$

we then obtain an implicit equation for the ground-state densities $\rho_{\mathrm{gs},\lambda,\sigma}$.

For convenience, let us consider identical fermions, that means all fermions have equal spin:

$$\rho_{\mathrm{gs},\lambda}(\chi) = -\frac{1}{\lambda}\int_{\chi_1} U^{-1}(\chi,\chi_1)\left(\left.\frac{\delta\Gamma_{\lambda=0}[\rho]}{\delta\rho(\chi_1)}\right|_{\rho_{\mathrm{gs},\lambda}}\right). \tag{3.89}$$

This is an implicit equation for the density $\rho_{\mathrm{gs},\lambda}$. Expanding the initial effective action $\Gamma_{\lambda=0}[\rho]$ about the initial ground-state $\rho_{\mathrm{gs},0} \equiv \rho_{\mathrm{gs},\lambda=0}$ up to second order, we find the following solution for $\rho_{\mathrm{gs},\lambda}$:

$$\rho_{\mathrm{gs},\lambda}(\chi) = \int_{\chi_1}\int_{\chi_2}\left[\lambda\,U + \Gamma^{(2)}_{\mathrm{gs},0}\right]^{-1}(\chi,\chi_1)\,\Gamma^{(2)}_{\mathrm{gs},0}(\chi_1,\chi_2)\,\rho_{\mathrm{gs},0}(\chi_2)\,, \tag{3.90}$$

where $\Gamma^{(2)}_{\mathrm{gs},0} := \Gamma^{(2)}_{\mathrm{gs},\lambda=0}[\rho_{\mathrm{gs},\lambda=0}]$. However, such a low-order expansion in ρ underlying the *Hartree* approximation can only be meaningful if the interacting ground-state $\rho_{\mathrm{gs},\lambda=1}$ is close to the initial non-interacting ground-state $\rho_{\mathrm{gs},\lambda=0}$. In general, it is difficult to judge *a priori* whether this is the case.[5] From a practical point of view, we

[5] Strictly speaking, the notion 'close' requires the definition of a measure on the space defined by the functions ρ. We shall skip this issue here.

therefore have to include higher orders in the expansion of $\Gamma_{\lambda=0}[\rho]$ and analyze the convergence of the physical observables as a function of the expansion order.

From Eq. (3.90), it follows that the *Hartree* approximation already yields arbitrarily high orders in an expansion in powers of $\bar{g}$, both for the ground-state energy and density. Recall that $U \sim \bar{g}$ and $E_{\mathrm{gs}} \sim \Gamma[\rho_{\mathrm{gs}}]$. However, we would like to point out a shortcoming of the *Hartree* approximation which becomes apparent from our analysis. Taking into account our findings from Sect. 3.4, we conclude that the *Hartree* approximation in general fails to reproduce the perturbative result for the ground-state energy, even at leading order. This is simply due to the fact that the second term on the right-hand side of Eq. (3.35) is missing in this approximation. This term depends explicitly on the interaction potential. Since $\delta^2\Gamma_\lambda/(\delta\rho\,\delta\rho)$ is in general not identical to zero, even in the non-interacting limit, this term generates terms which already contribute to the leading order in a perturbative expansion.

3.6 Variational Principle and Conventional DFT

DFT is built on the *Rayleigh-Ritz* variational principle, meaning that the exact density functional Γ is minimal at the exact ground-state density, where it is equal to the exact ground-state energy. Any other density plugged into the exact density functional Γ would result in a higher energy. The question on hand is now if the energy obtained from any given truncation of our set of RG flow equations is also always greater than the exact energy. As we will see in this section, this is not necessarily the case.

Let us consider again the flow equation for the ground-state energy as it follows from Eq. (3.71):

$$\begin{aligned}\partial_\lambda E_\lambda \equiv \partial_\lambda \langle \hat{H}\rangle_\lambda =& \frac{1}{2}\sum_{\sigma_1\sigma_2}\int_{x_1}\int_{x_2} n_{\mathrm{gs},\lambda,\sigma_1}(x_1)\,U_{\sigma_1\sigma_2}(x_1,x_2)\,n_{\mathrm{gs},\lambda,\sigma_2}(x_2)\\ &+\frac{1}{2}\sum_{\sigma_1\sigma_2}\int_{x_1}\int_{x_2} U_{\sigma_1\sigma_2}(x_1,x_2)\Big(G^{(2)}_{\lambda,\sigma_1\sigma_2}(0,x_1,0,x_2) - n_{\mathrm{gs},\lambda,\sigma_2}(x_2)\,\delta_{\sigma_2,\sigma_1}\,\delta(x_2-x_1)\Big)\,.\end{aligned} \tag{3.91}$$

Using the relation (3.48) between the density-density correlation function and the absolute square of the ground-state wavefunction, we obtain

$$\partial_\lambda E_\lambda \equiv \partial_\lambda \langle \hat{H}\rangle_\lambda = \frac{1}{2}\sum_{\sigma_1\sigma_2}\int_{x_1}\int_{x_2} U_{\sigma_1\sigma_2}(x_1,x_2)\,N_{\sigma_1}(N_{\sigma_2}-\delta_{\sigma_1,\sigma_2})\int_{x_3}\cdots\int_{x_N}|\Psi_{\mathrm{gs},\lambda}(x_1,\sigma_1,\ldots,x_N,\sigma_N)|^2 = \langle\hat{U}\rangle_\lambda\,, \tag{3.92}$$

where the subscript λ refers to the fact that the ground-state wavefunction in general depends on λ. Thus, we recover the *Hellmann-Feynman* theorem from the DFT-RG equation for the ground-state energy, if we choose the regulator $\mathscr{R}_\lambda(\tau,x,\tau',x') = \lambda$.

An integration of Eq. (3.92) with respect to λ eventually yields the ground-state energy:

$$\langle\hat{H}\rangle = E_{\lambda=0} + \frac{1}{2}\sum_{\sigma_1\sigma_2}\int_{x_1}\int_{x_2} U_{\sigma_1\sigma_2}(x_1,x_2)\,N_{\sigma_1}(N_{\sigma_2}-\delta_{\sigma_1,\sigma_2})\int_0^1 \mathrm{d}\lambda\int_{x_3}\cdots\int_{x_N}|\Psi_{\mathrm{gs},\lambda}(x_1,\sigma_1,\ldots,x_N,\sigma_N)|^2\,, \tag{3.93}$$

where the first term on the right-hand side is the energy of the non-interacting fermions. Hence, the ground-state energy can either be calculated from $|\Psi_{\mathrm{gs},\lambda}(x_1,\sigma_1,\ldots,x_N,\sigma_N)|^2$ or, equivalently, from the reduced quantity $\Phi_{N,\lambda,\sigma_1\sigma_2}$ which follows from $|\Psi_{\mathrm{gs},\lambda}(x_1,\sigma_1,\ldots,x_N,\sigma_N)|^2$ by integration over the coordinates x_i with $i=3,\ldots,N$, see Eq. (3.48). It is obvious that $\langle\hat{H}\rangle$ on the left-hand side of Eq. (3.93) should only be identified with the exact ground-state energy of the system, i. e. the expectation value of $\hat{H}$ with respect to the exact ground-state wavefunction, if $\Phi_{N,\lambda,\sigma_1\sigma_2}$ is exact, which implies that the infinite tower of RG flow equations for the correlation functions has been solved exactly. As discussed in Sec. 3.2, the change of $|\Psi_{\mathrm{gs},\lambda}(x_1,\sigma_1,\ldots,x_N,\sigma_N)|^2$

under a variation of λ can be extracted from the flow equation of the N-density correlation function $G^{(N)}_{\lambda,\sigma_1\ldots\sigma_N}$. Now we recall that the computation of the full λ-dependence of the correlation function $G^{(N)}_{\lambda,\sigma_1\ldots\sigma_N}$ requires the full λ-dependence of the correlation functions $G^{(m)}_{\lambda,\sigma_1\ldots\sigma_m}$ with $1 \leq m \leq N+2$. Of course, the associated infinite tower of flow equations for the correlation functions can in general not be solved without relying on approximations. For example, one may consider a truncation of this infinite tower to a finite set of flow equations, see also Chaps. 6 and 7. In any case, any truncation of this tower will in general yield only an approximate solution $\Phi^{(\mathrm{A,RG})}_{N,\lambda,\sigma_1\sigma_2}$ of $\Phi_{N,\lambda,\sigma_1\sigma_2}$. We may now ask whether the ground-state energy obtained from such an *approximate* solution is always greater than or equal to the exact ground-state energy. A necessary and sufficient condition for this to be the case is that an approximation $\Psi^{(\mathrm{A})}_{\mathrm{gs},\lambda}(x_1,\sigma_1,\ldots,x_N,\sigma_N)$ of the exact ground-state wavefunction can be constructed such that

$$\Phi^{(\mathrm{A,RG})}_{N,\lambda,\sigma_1\sigma_2}(x_1,x_2) = \int_{x_3}\cdots\int_{x_N} |\Psi^{(\mathrm{A})}_{\mathrm{gs},\lambda}(x_1,\sigma_1,\ldots,x_N,\sigma_N)|^2 \quad \text{and} \quad E^{(\mathrm{A,RG})}_{\lambda} = \langle\Psi^{(\mathrm{A})}_{\mathrm{gs},\lambda}|\hat{H}|\Psi^{(\mathrm{A})}_{\mathrm{gs},\lambda}\rangle \tag{3.94}$$

for $\lambda \in [0,1]$. Here, $E^{(\mathrm{A,RG})}_{\lambda}$ denotes the approximate DFT-RG result for the ground-state energy as obtained from $\Phi^{(\mathrm{A,RG})}_{N,\lambda}(x_1,x_2)$ where the latter has been obtained from a given truncation of the underlying infinite tower of flow equations. Indeed, the condition (3.94) implies

$$E^{(\mathrm{A,RG})}_{\lambda} \geq \langle\hat{H}\rangle\big|_{\mathrm{exact}} \tag{3.95}$$

according to the *Rayleigh-Ritz* variational principle. In particular, the condition (3.94) implies that the approximate wavefunction $\Psi^{(\mathrm{A})}_{\mathrm{gs},\lambda}(x_1,\sigma_1,\ldots,x_N,\sigma_N)$ satisfies the *Hellmann-Feynman* theorem.

As we shall see in Sec. 6.3 we can construct an approximation within our DFT-RG framework which corresponds to the *Hartree-Fock* approximation. Hence, in this case, the approximate ground-state wavefunction $\Psi^{(\mathrm{A})}_{\mathrm{gs},\lambda}$, which fulfills the condition (3.94), is given by a *Slater* determinant built up from one-particle wavefunctions of the non-interacting theory. However, there also exists a simple example for an approximation scheme which potentially violates the condition (3.94): Assume that an approximation of the DFT-RG flow equations has been constructed such that $E^{(\mathrm{A,RG})}_{\lambda=1}$ agrees identically with the second-order result from perturbation theory (PT), $E^{(\mathrm{PT})} = E^{(0)} + \bar{g}E^{(1)} + \frac{1}{2}\bar{g}^2E^{(2)}$. The perturbative calculation requires the wavefunction $|\Psi^{(\mathrm{PT})}_{\mathrm{gs}}\rangle$ in the leading-order approximation as input,

$$|\Psi^{(\mathrm{PT})}_{\mathrm{gs}}\rangle = |\Psi_{\mathrm{gs},0}\rangle + \bar{g}|\delta\Psi_{\mathrm{gs}}\rangle\,. \tag{3.96}$$

Here, the index 0 refers to the non-interacting system. Computing the expectation value of $\hat{H}$ with respect to this wavefunction, we obtain

$$\langle\Psi^{(\mathrm{PT})}_{\mathrm{gs}}|\hat{H}|\Psi^{(\mathrm{PT})}_{\mathrm{gs}}\rangle = \langle\Psi_{\mathrm{gs},0}|\hat{H}|\Psi_{\mathrm{gs},0}\rangle + 2\bar{g}\langle\delta\Psi_{\mathrm{gs}}|\hat{H}|\Psi_{\mathrm{gs},0}\rangle + \bar{g}^2\langle\delta\Psi_{\mathrm{gs}}|\hat{H}|\delta\Psi_{\mathrm{gs}}\rangle\,. \tag{3.97}$$

Evidently, $\langle\Psi^{(\mathrm{PT})}_{\mathrm{gs}}|\hat{H}|\Psi^{(\mathrm{PT})}_{\mathrm{gs}}\rangle$ includes a term of order $\bar{g}^3$ because a factor $\bar{g}$ is included in the operator $\hat{U} = \hat{H} - \hat{T}$ and therefore $\langle\Psi^{(\mathrm{PT})}_{\mathrm{gs}}|\hat{H}|\Psi^{(\mathrm{PT})}_{\mathrm{gs}}\rangle$ and $E^{(\mathrm{PT})}$ are in general not identical. In particular, $\langle\Psi^{(\mathrm{PT})}_{\mathrm{gs}}|\hat{H}|\Psi^{(\mathrm{PT})}_{\mathrm{gs}}\rangle$ satisfies the *Rayleigh-Ritz* variational principle, whereas $E^{(\mathrm{PT})}$ may violate the associated variational bound, i. e., $E^{(\mathrm{PT})}$ is not necessarily greater than or equal to the exact ground-state energy. Coming back to our DFT-RG framework, this implies that a truncation, which has been constructed such that $E^{(\mathrm{A,RG})}_{\lambda=1}$ agrees identically with the perturbative result at, e. g., second order, does not necessarily satisfy the *Rayleigh-Ritz* variational principle and therefore it is in general also not possible to construct an approximate wavefunction $\Psi^{(\mathrm{A})}_{\mathrm{gs},\lambda}$ in this case which satisfies the condition (3.94).

From these considerations we conclude that the ground-state energy obtained from a given truncation of our set of RG flow equations for the correlation functions is not necessarily greater than or equal to the exact ground-state energy. Since truncations correspond to approximations of the energy density functional (or, equivalently, the exchange-correlation functional in the terminology of conventional DFT), this also holds for conventional DFT studies. With respect to the latter note that any truncation of the vertex expansion (3.16), in which we at least take

into account the three-density correlation function, generates terms of arbitrarily high orders in $(\rho - \rho_{\mathrm{gs}})$ when we solve the associated set of RG flow equations. This can be readily seen from the flow equation (3.35) for the density functional $\Gamma[\rho] \sim E[\rho]$ which can be rewritten in the following way:

$$\begin{aligned}\Gamma[\rho] =& \Gamma_0[\rho] + \frac{1}{2}\sum_{\sigma_1\sigma_2}\int_{\chi_1}\int_{\chi_2}\rho_{\sigma_1}(\chi_1)U_{2b,\sigma_1\sigma_2}(\chi_1,\chi_2)\rho_{\sigma_2}(\chi_2) \\ &+ \frac{1}{2}\sum_{\sigma_1\sigma_2}\int_0^1 \mathrm{d}\lambda \int_{\chi_1}\int_{\chi_2} U_{2b,\sigma_1\sigma_2}(\chi_1,\chi_2)\Big(\big(\Gamma_\lambda^{(2)}[\rho]\big)^{-1}_{\sigma_1\sigma_2}(\chi_2,\chi_1) - \rho(\chi_2)\delta(\chi_2-\chi_1)\Big)\,. \end{aligned} \tag{3.98}$$

Here, the first term on the right-hand side corresponds to the kinetic energy functional associated with the non-interacting initial system. Since the inverse of the second functional derivative of $\Gamma_\lambda[\rho] \sim E_\lambda[\rho]$ appears on the right-hand side of Eq. (3.98), it indeed follows that terms of arbitrarily high orders in $(\rho_\sigma - \rho_{\mathrm{gs},\sigma})$ are generated in the RG flow, even if a finite truncation of Γ_λ has been used initially.

The vertex expansion (3.16) should not be confused with the local density approximation. As a matter of fact, the formally exact flow equation (3.35) nevertheless constrains the potentially possible approximations for Γ_λ . We want to illustrate this in the case of identical fermions with a simple example. Consider an ansatz for Γ_λ which is of the type of a local density approximation (LDA):

$$\Gamma_\lambda[\rho] \approx \gamma_{0,\lambda} + \sum_{m=2}^{\infty}\frac{\gamma_{m,\lambda}}{m!}\int_\chi (\rho(\chi) - \rho_{\mathrm{gs},\lambda}(\chi))^m\,, \tag{3.99}$$

where the γ_m's are λ-dependent real-valued numbers. For a general interaction potential U_{2b} , we observe that this ansatz does not allow for a consistent solution of the flow equation (3.35). In fact, according to the flow equation (3.35), we have $\Gamma_\lambda^{(2)} \sim U_{2b}$. On the other hand, the ansatz (3.99) yields $\Gamma_\lambda^{(2)} \sim \delta(\chi_1 - \chi_2)$ which is in general only consistent with the flow equation (3.35) for an interaction potential of the form $U_{2b} \sim \delta(\chi_1 - \chi_2)$. Whereas an interaction potential of this form can in principle be meaningful for systems of fermions with an internal degree of freedom (such as spin), it is not for identical fermions due to the *Pauli* exclusion principle. In our studies below, we shall therefore always employ the full vertex expansion (3.16), i. e. we take into account the full dependence of the correlation functions on time-like and spatial coordinates.

In section 2.5 we already showed that the vertex expansion of E_{HK} (2.42) about the ground-state density n_{gs} can be recast into the gradient expansion (2.43). The energy density functional E_{HK} (2.14) in that case has been a functional of the time-*independent* density field $n(x)$ rather than of the time-dependent density field $\rho(\tau, x)$. Here, we consider a functional Γ_λ of the time-dependent density field $\rho(\tau, x)$. Also in this case, the vertex expansion (3.16) can be recast into a derivative expansion, which in the case of identical fermions can be written as follows:

$$\Gamma_\lambda[\rho] = g_\lambda^{(0)}[\rho] + \int_\tau\int_x g_\lambda^{(2,0)}(\rho)(\partial_\tau\rho(\tau,x))^2 + \int_\tau\int_x g_\lambda^{(2,1)}(\rho)(\partial_x\rho(\tau,x))^2 + \ldots\,, \tag{3.100}$$

provided that the many-body system under consideration is invariant under $\tau \to -\tau$ and time translations $\tau \to \tau + \tau_0$, where τ_0 defines an arbitrary shift in time direction. Again, an investigation of the validity of such an expansion is difficult for the same reasons as in the case of conventional DFT and its applicability therefore needs to be carefully examined.

In general, the projection of the functional $\Gamma_\lambda[\rho]$, which maps a time- and space-dependent function $\rho(\tau, x)$ into a real number, onto the functional $E_{\mathrm{HK}}[n]$, which maps a space-dependent function $n(x)$ into a real number, is highly non-trivial, even if both functionals are associated with the same ground state. However, a comparison of the definitions of the (ground-state) density ρ_{gs} (see Eq. (3.11)) and the density-density correlation function $G_\lambda^{(2)}$ (see Eq. (3.28)) with the corresponding quantities entering the computation of energy density functionals of the type of $E_{\mathrm{HK}}[n]$ (see Ref. [57]) suggests the following projection rule for the correlation functions:

$$G_{\mathrm{HK}}^{(m)}(x_1,\ldots,x_m) = \lim_{\beta\to\infty}\frac{1}{\beta}\int_{-\beta/2}^{\beta/2}\mathrm{d}\tau_1\cdots\int_{-\beta/2}^{\beta/2}\mathrm{d}\tau_m\, G_\lambda^{(m)}(\tau_1,x_1,\ldots,\tau_m,x_m)\,. \tag{3.101}$$

Assuming that this rule holds for any $m \in \mathbb{N}$, the correlation functions $E_{\mathrm{HK}}^{(m)}$ appearing in Eq. (2.38) can be computed from the time-dependent correlation functions $G_\lambda^{(m)}$. For $m = 2$, for example, we have $E_{\mathrm{HK}}^{(2)} \sim (G_{\mathrm{HK}}^{(2)})^{-1}$. From these considerations we conclude that the two functionals $E_{\mathrm{HK}}[n]$ and $\Gamma_\lambda[\rho]$ are in general not identical, although the ground-state density may in both cases be described by the time-independent density $n_{\mathrm{gs}}(x)$. As discussed in Sec. 3.2 it is possible to extract, e. g., energies of excited states, from the time-dependent correlation functions associated with an expansion of $\Gamma_\lambda[\rho]$ about the ground-state density. In this sense, the functional $\Gamma_\lambda[\rho]$ contains more information than the *Hohenberg-Kohn* energy density functional and should therefore be considered as a generalization of it. From a comparison of Eq. (2.27) evaluated at the ground-state density n_{gs} with Eq. (3.93), we deduce that, loosely speaking, a particular ansatz for $E_{\mathrm{xc}}[n_{\mathrm{gs}}]$ is associated with an approximation for $\langle \hat{U} \rangle$ which involves the absolute square of the ground-state wavefunction $|\Psi_{\mathrm{gs},\lambda}|^2$. In the limit of many fermions, an LDA-type ansatz for E_{xc} is often found to yield reasonable results for ground-state properties, even on a quantitative level. This may be traced back to the fact that the LDA is directly obtained from the equation of state of the associated many-body problem (in the thermodynamic limit). For few-body systems, on the other hand, an LDA ansatz for E_{xc} is in general not sufficient for an accurate computation of ground-state properties and more involved ansätze for E_{xc} are required. Within our DFT-RG approach, the problem of finding an appropriate ansatz for E_{xc} is replaced by the computation of the density correlation functions.

We close this discussion with a comment on the relation of our approach to the *Hellmann-Feynman* theorem, see also Eq. (3.92). First of all, we note that the *Hellmann-Feynman* theorem does not provide a recipe for the computation of the λ-dependent wavefunction. On the other hand, our RG approach provides us with a recipe for the computation of the λ-dependence of the absolute square of the ground-state wavefunction via its relation to the density correlation functions. In this sense, our DFT-RG approach may be viewed as an extension of the *Hellmann-Feynman* theorem allowing for a systematic computation of the λ-dependent absolute square of the ground-state wavefunction.

Finally, we note that in conventional DFT studies, the *Hellmann-Feynman* theorem serves as a starting point for the derivation of so-called coupling-constant integration methods which in principle allow to compute a representation of the exchange-correlation functional in terms of *Kohn-Sham* orbitals and eigenvalues [3]. Our DFT-RG approach does not rely on the computation of the latter. It rather relies on a hierarchy of correlation functions computed from a non-interacting but confined system which defines the starting point of the associated RG flow.

3.7 Fermion Self-Interactions

In conventional DFT, an infamous problem in the construction of density functionals is the potential appearance of spurious fermion self-interactions which need to be removed by, e. g., "counter terms" in order to remove the associated self-interaction energy spoiling the predictions for ground-state energies. For example, the *Hartree* term yields a finite contribution to the energy even for a system containing only a single fermion, see Eq. (3.87).

Our DFT-RG approach relies on expanding the density functional about the ground state rather than making a global ansatz of this functional. As we have shown above, this expansion about the ground state can even be related to many-body perturbation theory. We shall now see that this also allows us to keep the problem of spurious self-interactions systematically under control. Indeed, we already deduce from Eq. (3.92) that $\partial_\lambda E_\lambda = 0$ for $N = 1$. Thus, no fermion self-interactions are present if we solve the infinite tower of RG flow equations exactly. To be more precise, the derivation of Eq. (3.92) relies on Eq. (3.48) which, for $N = 1$, reduces to the following "sum rule":

$$G_\lambda^{(2)}(0, x_1, 0, x_2) - n_{\mathrm{gs},\lambda}(x_1)\,\delta(x_1 - x_2) + n_{\mathrm{gs},\lambda}(x_2)\,n_{\mathrm{gs},\lambda}(x_2) = 0\,, \tag{3.102}$$

where we omit spin-indices because for one particle there is obviously only one possible spin. In practice, a solution of the flow equations for the ground-state density and the density-density correlation function requires a truncation of the infinite coupled set of flow equations associated with the density correlation functions. Any given truncation of this set may result in a violation of the sum rule (3.102). In our explicit numerical studies below, we estimate the

strength of the violation of this sum rule by computing the ground-state energy of the one-fermion system which may be considered as a quality measure of the given truncation.

As we will also see when we discuss the relation of our DFT-RG approach to perturbation theory in more detail for the model studies below, these spurious self-interaction contributions are not present in our DFT-RG approach if we consider the solution of the flow equations order by order in the parameter $\bar{g}$. As discussed above, this is equivalent to conventional many-body perturbation theory where we do not encounter contributions from spurious fermion self-interactions to the ground-state energy. This observation helps to guide the construction of truncations within our present framework: If a truncation is constructed in this spirit such that it reproduces many-body perturbation theory exactly up to a given order, then the contributions from fermion self-interactions generated in the full RG flow on the level of this trunction also approach zero in the perturbatively accessible weak-coupling limit. Moreover, the truncation can be systematically improved by including higher-order corrections of the perturbative series. In contrast to such a construction of truncations of the energy density functional, the size of contributions from fermion self-interactions is *a priori* completely uncontrolled when we simply "guess" a truncation of the energy density functional and the systematic cancellation of these spurious contributions may be difficult.

4 Zero-Dimensional Toy Model

In this chapter we want to start with a first application of our DFT-RG approach. Therefore, we apply the formalism to the simplest example one can think of, namely the computation of an ordinary integral. This corresponds loosely speaking to a zero-dimensional field theory. Zero-dimensional models have been successfully used to also benchmark other field-theoretical methods in the past, see, e. g., Ref. [64].

In the zero-dimensional case it is possible to compute the partition function exactly and obtain the exact 2PPI effective action Γ. This allows us to compare the exact effective action with the one we can reconstruct from the n-point functions within our approach. This application has also been discussed in Ref. [22].

The quantities $S[\psi]$, $Z[J]$, $W[J]$ and $\Gamma[\rho]$ are no functionals but ordinary functions in zero dimensions. Nevertheless, we stick to the notations introduced in the previous chapter. The partition function corresponding to Eq. (3.3) is of the form

$$Z[J] \sim \int_{-\infty}^{\infty} \mathrm{d}\psi \, \mathrm{e}^{-S[\psi]+J\psi^2}, \tag{4.1}$$

where we again dropped the irrelevant normalization factor and

$$S[\psi] = \frac{1}{2}\omega^2 \psi^2 + \frac{g}{24}\psi^4. \tag{4.2}$$

The function $S[\psi]$ is the analogue to the classical action (3.1) and is chosen to be similar to the classical action of fermionic theories. We have set the background potential to $V = \omega^2/2$ corresponding to a harmonic trap. The second term in Eq. (4.2) describes a two-body interaction, where the interaction potential is given by $U = g/12$. The derivative terms in the action vanish because J and ψ are real-valued numbers in this case.

For $\bar{J} = J/\omega^2 \leq 1/2$, the partition function can be given in closed form:

$$Z[\bar{J}] \sim \frac{\sqrt{3-6\bar{J}}\, K_{1/4}\left(\frac{3(1-2\bar{J})^2}{4\bar{g}}\right) \mathrm{e}^{\frac{3(1-2\bar{J})^2}{4\bar{g}}}}{\sqrt{\bar{g}}} \equiv \mathrm{e}^{W[J]}, \tag{4.3}$$

where $\bar{g} = g/\omega^4$ is the dimensionless coupling and K_ν is the modified Bessel function of the second kind of order ν, see Ref. [65]. For $\bar{J} > 1/2$, the integral $Z[J]$ can still be computed analytically but has different form. As we are interested in the limit $J \to 0$ corresponding to the ground state of the system, it suffices to restrict on the case for $\bar{J} \leq 1/2$.

We continue with our study of the analytically solvable case for $\bar{J} = J/\omega^2 \leq 1/2$. In this zero-dimensional case, Eq. (3.12) simplifies to

$$\rho = \frac{\delta W[J]}{\delta J}, \tag{4.4}$$

and we can compute the ground-state 'density' $\rho_{\mathrm{gs}} \equiv \langle \psi^2 \rangle_{\mathrm{gs}}$ by taking the limit $J \to 0$:

$$\rho_{\mathrm{gs}} = \frac{\frac{3}{2} K_{5/4}\left(\frac{3}{4\bar{g}}\right) + \frac{3}{2} K_{-3/4}\left(\frac{3}{4\bar{g}}\right) - (\bar{g}+3)\, K_{1/4}\left(\frac{3}{4\bar{g}}\right)}{\omega^2\, \bar{g}\, K_{1/4}\left(\frac{3}{4\bar{g}}\right)}. \tag{4.5}$$

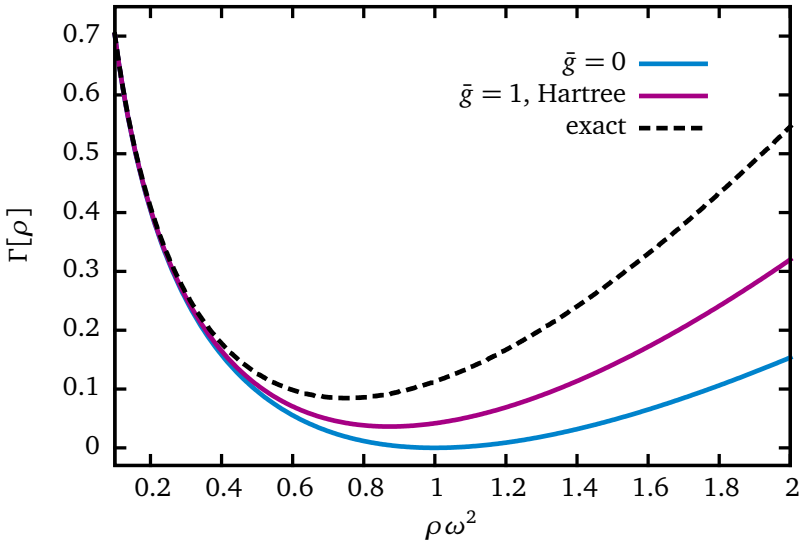

Figure 4.1.: Effective action $\Gamma[\rho]$ of the zero-dimensional toy model for the non-interacting case $\bar{g} = 0$ and for $\bar{g} = 1$, as obtained from a direct calculation of the partition function. We have normalized the effective action such that $\Gamma[\rho_{\mathrm{gs}}] = 0$ for $\bar{g} = 0$.

This expression can be expanded in powers of $\bar{g}$:

$$\rho_{\mathrm{gs}} = \omega^{-2}\left(1 - \frac{\bar{g}}{2} + \frac{2\,\bar{g}^2}{3} - \frac{11\,\bar{g}^3}{8} + \mathcal{O}\left(\bar{g}^4\right)\right). \tag{4.6}$$

The ground-state 'energy' can be obtained directly from

$$E_{\mathrm{gs}} = -\left(\ln Z[0] - \ln Z[0]\big|_{g\to 0}\right) \tag{4.7}$$

$$= -\ln\left(\frac{\sqrt{3}\,\mathrm{e}^{\frac{3}{4\bar{g}}}}{\sqrt{\bar{g}}} K_{1/4}\left(\frac{3}{4\,\bar{g}}\right)\right) + \frac{1}{2}\ln(2\pi), \tag{4.8}$$

where we have normalized E_{gs} such that it is zero for vanishing interaction, or $\bar{g} \to 0$. For small $\bar{g}$ we find

$$E_{\mathrm{gs}} = \frac{\bar{g}}{8} - \frac{\bar{g}^2}{12} + \frac{11\bar{g}^3}{96} + \mathcal{O}\left(\bar{g}^4\right) \tag{4.9}$$

and for large $\bar{g}$ we find $E_{\mathrm{gs}} \sim \ln(\bar{g})$.

Alternatively, we may compute the effective action $\Gamma[\rho]$ using Eq. (3.13). From a minimization of the effective action $\Gamma[\rho]$ we can then obtain E_{gs} and ρ_{gs}. To compute $\Gamma[\rho]$, Eq. (4.4) has to be solved for J. The solution $J \equiv J[\rho]$ needs to be plugged into the equivalent of the definition of the effective action (3.13) for the zero-dimensional case. We find

$$\Gamma[\rho] = -W[J[\rho]] + J[\rho]\,\rho\,. \tag{4.10}$$

For $\bar{g} = 0$ the effective action can be computed analytically:

$$\Gamma_{\bar{g}=0}[\rho] = \frac{1}{2}\left(\rho\omega^2 - \ln\left(2\pi\rho\omega^2\right) - 1\right). \tag{4.11}$$

Apparently, any polynomial ansatz for $\Gamma_{\bar{g}=0}$ is bound to fail. Note that γ is not analytic at $\rho = 0$. A Taylor expansion about the ground-state $\rho_{\mathrm{gs}}\omega^2 = 1$ (for $\bar{g} = 0$) is still possible and meaningful.

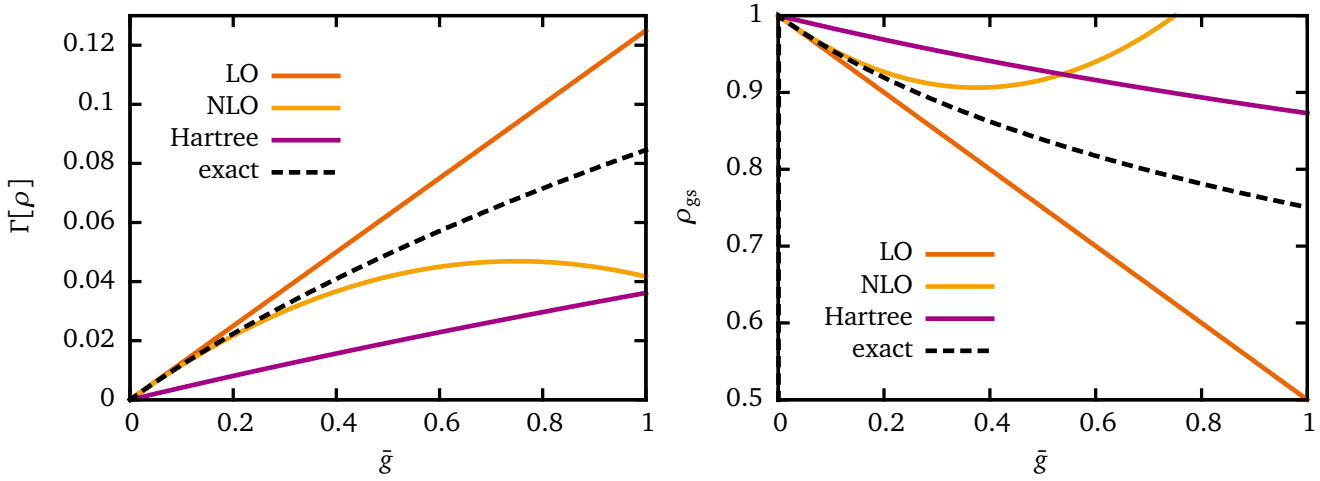

Figure 4.2.: Ground-state 'energy' E_{gs} and ground-state 'density' ρ_{gs} of the zero-dimensional toy model as a function of the (dimensionless) coupling $\bar{g}$. For comparison, we also show the results from a small-coupling expansion at leading order (LO) and next-to-leading order (NLO).

For $\bar{g} > 0$, the computation of the effective action can only be performed numerically. We find that the non-analyticity at $\rho = 0$ persists in this case. In Fig. 4.1 we show the effective action $\Gamma[\rho]$ as a function of ρ for $\bar{g} = 1$. We have normalized $\Gamma[\rho]$ such that $\Gamma[\rho_{\mathrm{gs}}] = 0$ for $\bar{g} = 0$. For $\bar{g} = 1$, the ground state ρ_{gs} is found at $\rho_{\mathrm{gs}} \approx 0.7505$, in agreement with our analytic result (4.5). For the ground-state 'energy', we find $E_{\mathrm{gs}} \approx 0.0846$ which also agrees with the value analytically found from Eq. (4.8).

We can compare these results with those from the effective action in the *Hartree* approximation as derived from Eq. (3.87):

$$\Gamma_{\mathrm{Hartree}}[\rho] = \frac{\bar{g}}{24}(\rho\omega^2)^2 + \Gamma_{\bar{g}=0}[\rho] + \frac{1}{2}\ln(2\pi)\,. \tag{4.12}$$

The normalization has been again chosen such that $\Gamma_{\mathrm{Hartree}}[\rho_{\mathrm{gs,Hartree}}] = 0$ for $\bar{g} \to 0$. For the ground state we find

$$\begin{aligned}\rho_{\mathrm{gs,Hartree}}(\bar{g}) &= \bar{g}^{-1}\left(\sqrt{6\bar{g}+9} - 3\right) \\ &= 1 - \frac{\bar{g}}{6} + \frac{\bar{g}^2}{18} - \frac{5\bar{g}^3}{216} + \mathcal{O}\left(\bar{g}^4\right).\end{aligned} \tag{4.13}$$

The ground-state energy is then given by

$$\begin{aligned}E_{\mathrm{gs,Hartree}}(\bar{g}) &= \Gamma_{\mathrm{Hartree}}[\rho_{\mathrm{gs,Hartree}}] \\ &= \frac{\bar{g}}{24} - \frac{\bar{g}^2}{144} + \frac{5\bar{g}^3}{2592} + \mathcal{O}\left(\bar{g}^4\right).\end{aligned} \tag{4.14}$$

Clearly, the *Hartree* approximation does not reproduce the exact results, even in the small-coupling limit. In fact, it significantly underestimates the exact results for E_{gs} and overestimates those for the ground-state ρ_{gs}. In Fig. 4.2 the results for E_{gs} and ρ_{gs} from the exact small-coupling expansion and the *Hartree* approximation are compared to the exact results. In Fig. 4.1, we also show the effective action $\Gamma[\rho]$ in the *Hartree* approximation for comparison.

For illustration purposes, we now compute E_{gs} and ρ_{gs} in our DFT-RG approach. In this chapter we want to get a feeling for the quality of the vertex-type expansion of the effective action Γ, therefore we focus on the flow equation for Γ, see Eq. (3.35). In the present case, it assumes a simple form:

$$\partial_\lambda \Gamma_\lambda[\rho] = \frac{1}{24}\bar{g}\omega^4\left[\rho^2 + \left(\frac{\delta\Gamma_\lambda[\rho]}{\delta\rho\delta\rho}\right)^{-1}\right]. \tag{4.15}$$

In order to solve this equation, we expand $\Gamma[\rho]$ about the current ground-state $\rho_{\mathrm{gs},\lambda}$, see also Eq. (3.16):

$$\Gamma_\lambda[\rho] = \Gamma_\lambda[\rho_{\mathrm{gs},\lambda}] + \sum_{n=2}^{N_{\max}} \frac{1}{n!} \Gamma_\lambda^{(n)}[\rho_{\mathrm{gs},\lambda}](\rho - \rho_{\mathrm{gs},\lambda})^n , \tag{4.16}$$

where $N_{\max}$ denotes the order of the truncation. Note that $\partial_\lambda \Gamma_\lambda^{(1)}[\rho_{\mathrm{gs},\lambda}] \equiv 0$ and $\Gamma_{\lambda=0}^{(1)}[\rho_{\mathrm{gs},\lambda}] \equiv 0$ by definition. It is possible to choose different types of truncations. Plugging the expansion (4.16) into the flow equation (4.15) yields a tower of flow equations for $E_{\mathrm{gs},\lambda} = \Gamma_\lambda[\rho_{\mathrm{gs},\lambda}]$, $\rho_{\mathrm{gs},\lambda}$, and the n-point functions $\Gamma_\lambda^{(n)}[\rho_{\mathrm{gs},\lambda}]$. The initial conditions for these flow equations can be extracted by expanding $\Gamma_{\bar{g}=0}[\rho]$ about its ground-state density ρ_{gs}. Here, we want to focus on two possibilities.

For the first kind of truncation (RG-A1) we expand both sides of Eq. (4.15) to the same order in the expansion (4.16). For a given $N_{\max}$ we obtain flow equations for E_{gs}, ρ_{gs} and the n-point functions $\Gamma_\lambda^{(n)}[\rho_{\mathrm{gs}}]$ with $n \leq N_{\max}$. As discussed in the previous chapter, the flow equations for the n-point functions $\Gamma_\lambda^{(n)}$ depend in principle on the m-point functions $\Gamma_\lambda^{(m)}$ with $m \leq n+2$. For this truncation we neglect the terms containing n-point functions with $m = n+1$ and $m = n+2$. For $N_{\max} = 2$, for example, we find the following set of coupled ordinary first-order differential equations:

$$\partial_\lambda E_{\mathrm{gs},\lambda} = \frac{1}{24} \bar{g} \omega^4 \left[\rho_{\mathrm{gs},\lambda}^2 + \left(\Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda}] \right)^{-1} \right], \tag{4.17}$$

$$\partial_\lambda \rho_{\mathrm{gs},\lambda} = -\frac{1}{12} \bar{g} \omega^4 \rho_{\mathrm{gs},\lambda} \left(\Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda}] \right)^{-1}, \tag{4.18}$$

$$\partial_\lambda \Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda}] = \frac{1}{12} \bar{g} \omega^4 . \tag{4.19}$$

Note that $N_{\max} = 2$ is sufficient to exactly reproduce the perturbative results for the ground-state energy E_{gs} at leading order. In order to correctly reproduce the leading-order of the perturbative expansion of the ground state ρ_{gs} and the n-point functions at higher order, we need to increase the truncation order beyond $N_{\max} = 2$. From our general discussion in Chap. 3, it follows that $N_{\max} = 4$ is sufficient to correctly reproduce the perturbative series of ρ_{gs} and $\Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda}]$ at leading order. Moreover, we also recover the correct results for E_{gs} at next-to-leading order with $N_{\max} = 4$.

The set of flow equations for $N_{\max} = 2$ can be solved analytically and we find

$$E_{\mathrm{gs}}(\bar{g}) = \frac{1}{4} \left(\frac{\bar{g}}{6+\bar{g}} + 2 \ln \left(\frac{6+\bar{g}}{6} \right) \right) \sim \ln \bar{g} . \tag{4.20}$$

This is in accordance with the asymptotic behavior of the exact result, only that the coefficient of this term is not reproduced correctly for $N_{\max} = 2$.

The second kind of truncation (RG-A2) we discuss here uses the full flow equations for the n-point functions $\Gamma_\lambda^{(n)}$ up to a given order $N_{\max}$. All flow equations for higher-order n-point functions are neglected. Since the n-point functions with $n = N_{\max}+1$ and $n = N_{\max}+2$ also contribute to the considered flow equations, they are set to their initial values in the set of considered equations, i. e., we replace $\Gamma_\lambda^{(N_{\max}+1)} \to \Gamma_{\lambda=0}^{(N_{\max}+1)}$ and $\Gamma_\lambda^{(N_{\max}+2)} \to \Gamma_{\lambda=0}^{(N_{\max}+2)}$ in the flow equations of $\Gamma_\lambda^{(N_{\max}-1)}$ and $\Gamma_\lambda^{(N_{\max})}$. For this truncation scheme we can also define a flow equation for $N_{\max} = 1$ which identically reproduces first-order perturbation theory. The problem then reduces to the flow equation for the energy

$$\partial_\lambda E_{\mathrm{gs},\lambda} = \frac{1}{24} \bar{g} \omega^4 \left[\rho_{\mathrm{gs},\lambda=0}^2 + \left(\Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda=0}] \right)^{-1} \right]. \tag{4.21}$$

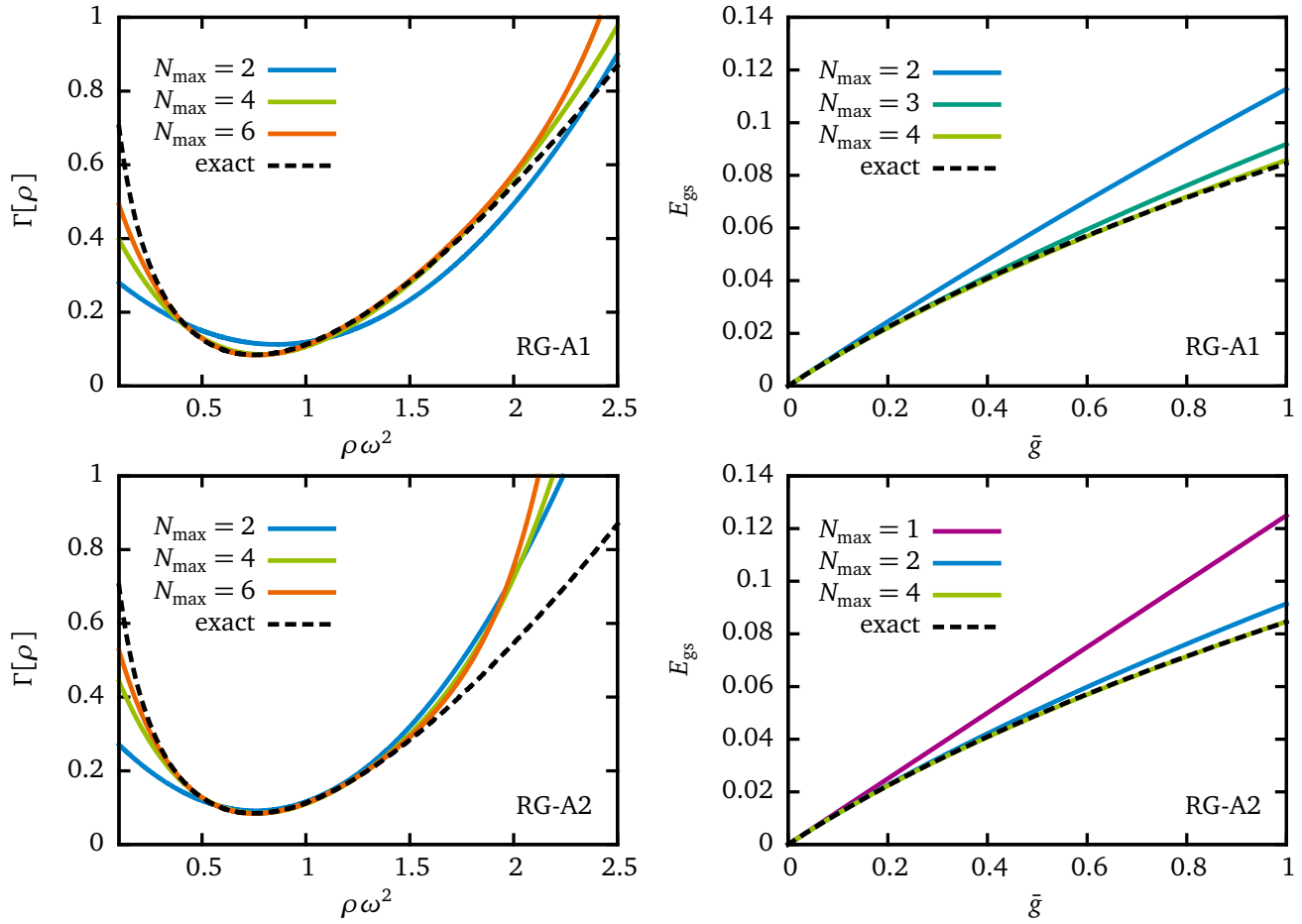

Figure 4.3.: Effective action $\Gamma[\rho] \equiv \Gamma_{\lambda=1}[\rho]$ and ground-state energy E_{gs} of the zero-dimensional toy model as obtained from our RG approach for various values of $N_{\max}$ for fixed $\bar{g} = 1$. We have normalized the effective action such that $\Gamma_{\lambda=1}[\rho_{\mathrm{gs}}] = 0$ for $\bar{g} = 0$. In the first row the result for the first discussed truncation (RG-A1) are shown. In the second row the results from the second truncation (RG-A2) can be found. Note that our results for the energy for $N_{\max} = 4$ are already almost indistinguishable from the exact values for E_{gs} on the scale of the plot for both truncations.

This can be solved analytically and we find $E_{\mathrm{gs}} = \bar{g}/8$ in accordance with the first-order perturbative result, see Eq. (4.9). For $N_{\max} = 2$ we find the following set of coupled differential equations:

$$\partial_\lambda E_{\mathrm{gs},\lambda} = \frac{1}{24}\bar{g}\omega^4\left[\rho_{\mathrm{gs},\lambda}^2 + \left(\Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda}]\right)^{-1}\right], \tag{4.22}$$

$$\partial_\lambda \rho_{\mathrm{gs},\lambda} = -\frac{1}{24}\bar{g}\omega^4\left[\rho_{\mathrm{gs},\lambda}\left(\Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda}]\right)^{-1} - \left(\Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda}]\right)^{-3}\Gamma_{\lambda=0}^{(3)}[\rho_{\mathrm{gs},\lambda=0}]\right], \tag{4.23}$$

$$\begin{aligned}\partial_\lambda \Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda}] = \frac{1}{24}\bar{g}\omega^4\Big[2 - \rho_{\mathrm{gs},\lambda}\left(\Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda=0}]\right)^{-1}\Gamma_{\lambda=0}^{(3)}[\rho_{\mathrm{gs},\lambda=0}] + 3\left(\Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda}]\right)^{-3}\left(\Gamma_{\lambda=0}^{(3)}[\rho_{\mathrm{gs},\lambda=0}]\right)^2 \\ -\left(\Gamma_\lambda^{(2)}[\rho_{\mathrm{gs},\lambda}]\right)^{-2}\Gamma_{\lambda=0}^{(4)}[\rho_{\mathrm{gs},\lambda=0}]\Big],\end{aligned} \tag{4.24}$$

where we used the initial conditions $\Gamma_{\lambda=0}^{(3)}$ and $\Gamma_{\lambda=0}^{(4)}$. With this truncation we recover the exact result for E_{gs} at next-to-leading-order and the exact result for E_{gs} at next-to-next-to-leading-order with $N_{\max} = 4$.

No matter which truncation scheme we choose, we can in both cases use the results for the n-point functions obtained by solving the flow equations to find an approximation for the density functional $\Gamma_\lambda[\rho]$. To this end, we plug the approximated n-point functions into the expansion (4.16).

In the left panel of Fig. 4.3, we present our results for $\Gamma[\rho] \equiv \Gamma_{\lambda=1}[\rho]$ as a function of ρ for various values of $N_{\max}$ for fixed $\bar{g} = 1$ for both truncation schemes, compared to exact results. Note that the radius of convergence r_ρ of

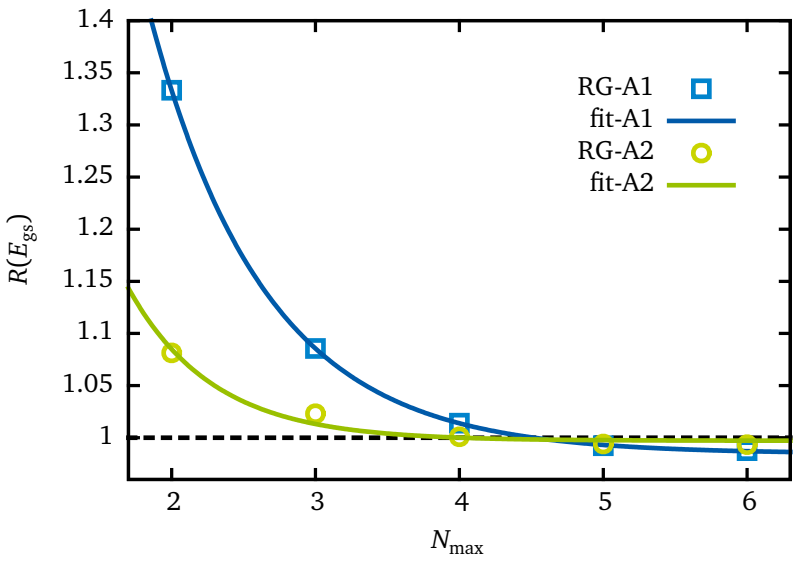

Figure 4.4.: $R(E_{gs}) = E_{gs}^{RG}/E_{gs}^{exact}$ as a function of N_{max} for $\bar{g} = 1$. The solid lines represent a fit of the RG data to the empirical ansatz (4.25), see main text for more details.

our expansion (4.16) about the ground state is finite. In fact, we find $r_\rho/\omega^2 = 1$ for the (dimensionless) radius of convergence in the case $\bar{g} = 0$. Our numerical results for finite $\bar{g}$ are in accordance with this result. In fact, we do not observe a convergent behavior around $\rho\omega^2 \approx 2$ for increasing N_{max}. For the second truncation scheme (RG-A2), the radius of convergence seems to be even smaller than in the first case. On the other hand, our results for $\Gamma[\rho]$ nicely approach the exact results for $|\rho - \rho_{gs}|\omega^2 \lesssim 1$ when N_{max} is increased for both truncation schemes. In order to compute $\Gamma[\rho]$ for $\rho\omega^2 > 2$, we could employ Taylor expansions around various different points with overlapping regions of convergence. This would be of importance, for example, when we expect that $\Gamma[\rho]$ develops various minima. As we are here only interested in computing the ground-state properties of the present system we conclude that both truncation schemes seem to converge nicely at the minimum corresponding to $\rho_{gs,\lambda}$.

In the right panel of Fig. 4.3, we present our RG results for E_{gs} as a function of $\bar{g}$ for various values for N_{max}. For both truncation schemes we find that our results for $N_{max} = 4$ are already in very good agreement with the exact results for $\bar{g} \lesssim 1$ and that we approach the exact results from above for increasing N_{max}. For values of the coupling $\bar{g} > 1$, we observe that we need to go to higher truncation orders in order to reproduce the exact results. Assuming that we do not know the exact solution for a given value of $\bar{g}$, these findings imply that we have to compute E_{gs} as a function of N_{max} and check numerically the convergence of this function. This is illustrated for $\bar{g} = 1$ in Fig. 4.4. The solid lines show the result from a fit of the RG data for $N_{max} = 2, 3, 4, 5, 6$ to the (empirical) three-parameter ansatz

$$E_{gs}^{RG}(N_{max}) = E_{gs}^{fit} + \alpha_1 e^{-\alpha_2 N_{max}}. \tag{4.25}$$

Here, E_{gs}^{fit}, α_1, and α_2 are the three fit parameters. For the first truncation we obtain $E_{gs}^{fit-A1} \approx 0.0833$ which is about 2% smaller than the exact result $E_{gs} \approx 0.0846$ and for the second truncation we obtain $E_{gs}^{fit-A2} \approx 0.0844$ which is about 1% smaller than the exact result.

This first analysis already exemplifies the application of our DFT-RG approach and shows how meaningful truncation schemes can be constructed to recover the exact solution of a given problem. In the next chapters, we shall use the discussed truncation schemes to study one-dimensional many-body systems.

5 Fermions in a One-Dimensional Box

To use our DFT-RG formalism we need to specify a background potential to confine the fermions in the initial non-interacting system. In this thesis we want to study systems of identical fermions, see Chap. 6, and systems of spin-$^1/_2$ fermions, see Chap. 7.

The flow equations introduced in Chap. 3 describe the change of the energy density functional or the generating functional of the connected correlation functions, respectively, under gradual changes of the interaction. The starting point for the RG flow is given by a system of confined but non-interacting fermions. If we aim at a study of the formation of selfbound systems, it is convenient to confine the fermions in a box with extent L that keeps the system bound in the RG flow. The limit $L \to \infty$ is then eventually taken at the end of the flow, i. e., when the interaction has been fully turned on.

In this chapter we now specify the setup we will use in the following two chapters and introduce the boundary conditions we have chosen. Since in general translation invariance is broken in a finite box, even if the potential only depends on $|x_1 - x_2|$, we introduce a periodically extended potential, to impose translation invariance also in the presence of the box.

We will give the initial conditions of our flow equations, i. e. the energy, density and the density correlation functions of the non-interacting system. Moreover, we use the specifications made in this chapter to investigate which simplifications of the flow equations for the density and the density correlation functions can be found.

5.1 Setup and Boundary Conditions

We choose a box with extent L for the confining potential. Therefore, we need first of all to specify the boundary conditions. Since we are aiming at the continuum limit, the box does not have a physical meaning in our case, hence the choice of the boundary conditions is at our disposal. Here, we choose periodic boundary conditions for fermions with spin σ if the number of spin-σ fermions N_σ is odd and antiperiodic boundary conditions for fermions with spin σ if the number of spin-σ fermions N_σ is even. This ensures that the ground state of the free gas of the $N = \sum_\sigma N_\sigma$ fermions, i. e. the starting point of the RG flow, is not degenerate. In systems with an even number of fermions with spin σ and an odd number of fermions with spin σ' fermions with different spins obey different boundary conditions. The possible fermion momenta are then given by

$$p_n^{(\mathrm{P})} = \frac{2\pi n}{L} \tag{5.1}$$

for odd numbers of particles and by

$$p_n^{(\mathrm{A})} = \frac{(2n+1)\pi}{L} \tag{5.2}$$

for even numbers of particles with $n \in \mathbb{Z}$, see Fig. 5.1 for an illustration. We emphasize that, in both cases, the density correlation functions being built up from one-particle propagators obey periodic boundary conditions. This follows from the fact that the density operator is given by $\hat{n}_\sigma(x) \sim \hat{\psi}_\sigma^\dagger(x)\hat{\psi}_\sigma(x)$. Thus, the associated one-particle wavefunctions and their complex conjugates enter the correlation functions always pairwise, leaving us with periodic boundary conditions for these functions in either case. However, the fact that the density correlation functions obey periodic boundary conditions is quite convenient since this allows us to rewrite these functions in terms of a Fourier series straightforwardly and it does not introduce an additional artificial breaking of translation invariance.

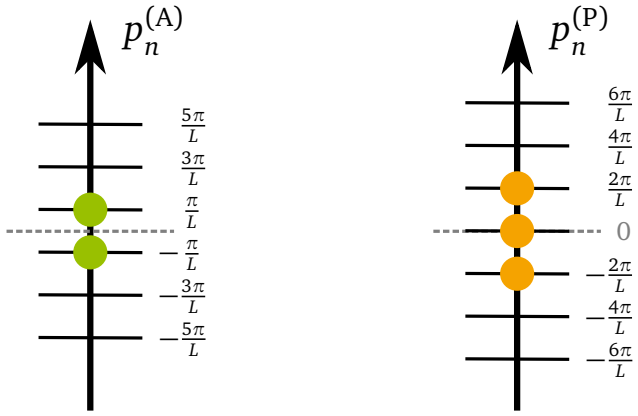

Figure 5.1.: Ground-state configuration of two fermions with equal spin in a box with finite extent L and antiperiodic boundary conditions (left-hand side) as well as the ground-state configuration of three fermions with equal spin in a box with periodic boundary conditions (right-hand side).

In the definition of the classical action (3.1) we have included a potential V which describes the box with extent L. In practice, the fermion-confining potential is not included explicitly in the calculations. Instead, we restrict the quantum fields on the domain $[-L/2, L/2)$ and impose appropriate boundary conditions. Therefore, we will use the shorthand $\int_x = \int_{-L/2}^{L/2} \mathrm{d}x$ in this chapter and in Chaps. 6 and 7.

Translational invariance is broken in the presence of a finite box. To embed translational invariance we redefine the interaction potential U in such a way that, for $|x_1 - x_2| \leq L/2$, U is still identical to the original interaction potential in the infinite-volume limit but obeys the periodicity condition

$$U(x_1 - x_2 + mL) = U(x_1 - x_2) \tag{5.3}$$

for $|x_1 - x_2| > L$ with $m \in \mathbb{Z}$. Note that we implement this periodically extended potential just for convenience and that our DFT-RG approach does not require to impose periodicity of the interaction in the presence of the box but works with any type of interaction. The so-defined two-body potential $U(x)$ depends only on $|x_1 - x_2|$ even for finite L and is a continuous periodic function of x on the interval $[-L/2, L/2)$, which is convenient for numerical studies of the DFT-RG flow equations. Apparently, our *redefined* interaction potential is not identical to the original interaction in the presence of the box. However, it approaches the original interaction potential in the infinite-volume limit which is of most relevance for a study of the formation of selfbound states in the absence of this auxiliary fermion-confining box.[1]

To derive the initial conditions and solve the flow equations it is convenient to write the one-particle propagator, the density correlation functions and the interaction potential as an expansion in terms of the one-particle eigenstates of the box. The position-space representations of the latter are given by

$$\begin{aligned} \phi_n^{(I_\sigma)}(x) = \frac{1}{\sqrt{L}} \mathrm{e}^{-\mathrm{i}p_n^{(I_\sigma)}x} \quad \text{with} \quad \int_x (\phi_m^{(I_\sigma)}(x))^* \phi_n^{(I_\sigma)}(x) = \delta_{m,n} \\ \text{and} \quad \sum_n (\phi_n^{(I_\sigma)}(x_1))^* \phi_n^{(I_\sigma)}(x_2) = \sum_n \delta(x_1 - x_2 + nL), \end{aligned} \tag{5.4}$$

where $n, m \in \mathbb{Z}$ and $I_\sigma \in \{\mathrm{P}, \mathrm{A}\}$, see Eqs. (5.1) and (5.2). For the one-particle propagator $\Delta_{\lambda=0,\sigma}^{(I_\sigma)}$ we use $I_\sigma = \mathrm{P}$ if N_σ is odd and $I_\sigma = \mathrm{A}$ if N_σ is even. For the expansion of the density correlation functions we always use $I_\sigma = \mathrm{P}$, because these functions obey periodic boundary conditions in every case, as already mentioned before.

[1] By solving the two-body problem exactly for both definitions of the interaction in the box, we have checked that the correct infinite-volume limit is indeed recovered, see App. B.2.

The Fourier-series representation of the "original" interaction potential U is given by

$$U_{\sigma_1\sigma_2}(x_1-x_2) = g\sum_{m,n} \mathfrak{U}^{m,n}_{\sigma_1\sigma_2} (\phi^{(\mathrm{P})}_m(x_1))^* \phi^{(\mathrm{P})}_n(x_2)\,. \tag{5.5}$$

Due to the redefinition of the potential, only the diagonal elements are needed to expand the potential, which means that for the periodically extended potential the following relation holds:

$$\mathfrak{U}^{m,n}_{\sigma_1\sigma_2} = \mathfrak{U}^{m,m}_{\sigma_1\sigma_2}\delta_{m,n}\,. \tag{5.6}$$

We would like to mention that at least the leading-order perturbative correction of the energy depends only on the diagonal elements of the matrix $\mathfrak{U}^{m,n}_{\sigma_1\sigma_2}$ anyways, as we will see below. Note that in general $\mathfrak{U}^{m,n}_{\sigma_1\sigma_2} \neq 0$ for $m \neq n$ and the "original" potential in a finite box, even if the interaction only depends on $|x_1-x_2|$. Thus, translational invariance is explicitly broken by the presence of the box.

5.2 Initial Conditions

We will now derive the initial conditions for our DFT-RG flow equations. The starting point of the DFT-RG flow is the non-interactiong system of N_σ spin-σ fermions and a total number of $N = \sum_\sigma N_\sigma$ fermions. The initial conditions, indicated by the index "$\lambda = 0$", are also the zeroth order of the perturbative expansion.

For the N-body system in a box with N_σ fermions of spin σ we find for the energy

$$E_{\lambda=0} = \sum_\sigma \sum_n \varepsilon^{(I_\sigma)}_n \theta(-\bar{\varepsilon}^{(I_\sigma)}_{\sigma,n}) = \sum_\sigma \frac{\pi^2}{6} N_\sigma \left(\frac{N_\sigma}{L}\right)^2 \left(1-\frac{1}{N_\sigma^2}\right), \tag{5.7}$$

where the one-particle energies are given by

$$\varepsilon^{(I_\sigma)}_n = \frac{1}{2}(p^{(I_\sigma)}_n)^2\,. \tag{5.8}$$

The auxiliary function θ is defined as follows

$$\theta(\pm\bar{\varepsilon}^{(I_\sigma)}_{\sigma,n}) = \begin{cases} 1 & \text{for} \quad \pm\bar{\varepsilon}^{(I_\sigma)}_{\sigma,n} \mp \eta > 0\,, \\ 0 & \text{otherwise}\,. \end{cases} \tag{5.9}$$

Here, $\eta \to 0^+$ is tacitly assumed. Moreover, we have introduced $\bar{\varepsilon}^{(I_\sigma)}_{\sigma,n} = \varepsilon^{(I_\sigma)}_n - \varepsilon^{(I_\sigma)}_{\mathrm{F},\sigma}$, where the Fermi energies

$$\varepsilon^{(\mathrm{A})}_{\mathrm{F},\sigma} = \varepsilon^{(\mathrm{A})}_{\frac{N_\sigma}{2}-1} \quad (N_\sigma \text{ even}) \quad \text{and} \quad \varepsilon^{(\mathrm{P})}_{\mathrm{F},\sigma} = \varepsilon^{(\mathrm{P})}_{\frac{N_\sigma-1}{2}} \quad (N_\sigma \text{ odd}) \tag{5.10}$$

are determined by the number of spin-σ fermions N_σ. The initial energy is given by the sum of the N_σ lowest one-particle energies of every spin species in the system. Note that the expression on the right-hand side of Eq. (5.7) depends only on N_σ and L but not on the choice of the boundary conditions.

For the one-particle propagator as defined in Eq. (3.24), we find the following expression for the one-paricle states of a non-interacting system in a box with (anti)periodic boundary conditions:

$$\begin{aligned}
&\Delta^{(I_\sigma)}_{\lambda=0,\sigma}(\tau_1,x_1,\tau_2,x_2) \\
&\quad = -\sum_n \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \frac{\mathrm{e}^{-\mathrm{i}\omega(\tau_1-\tau_2)}}{-\mathrm{i}\omega + \bar{\varepsilon}^{(I_\sigma)}_{\sigma,n}} (\phi^{(I_\sigma)}_n(x_1))^* \phi^{(I_\sigma)}_n(x_2) \\
&\quad = -\sum_n \Big\{\theta(\bar{\varepsilon}^{(I_\sigma)}_{\sigma,n})\theta_\tau(\tau_1-\tau_2) - \theta(-\bar{\varepsilon}^{(I_\sigma)}_{\sigma,n})\theta_\tau(\tau_2-\tau_1)\Big\} (\phi^{(I_\sigma)}_n(x_1))^* \phi^{(I_\sigma)}_n(x_2)\, \mathrm{e}^{-|\bar{\varepsilon}^{(I_\sigma)}_{\sigma,n}||\tau_1-\tau_2|}\,.
\end{aligned} \tag{5.11}$$

The basis functions $\phi_n^{(I_\sigma)}$ are defined in Eq. (5.4). From the one-particle propagator, we can now construct the initial conditions of the density as well as the density correlation functions. For the density, we find from Eq. (3.25) that

$$n_{\mathrm{gs},\lambda=0,\sigma}(x) \equiv \rho_{\mathrm{gs},\lambda=0,\sigma}(0,x) = \lim_{\tau\to 0^-} \Delta^{(I_\sigma)}_{\lambda=0,\sigma}(\tau,x,0,x) = \sum_n (\phi_n^{(I_\sigma)}(x))^* \phi_n^{(I_\sigma)}(x)\theta(-\bar{\varepsilon}^{(I_\sigma)}_{\sigma,n}) = \frac{N_\sigma}{L} \tag{5.12}$$

and

$$n^{(0)}_{\mathrm{gs}}(x) = \sum_\sigma n^{(0)}_{\mathrm{gs},\sigma}(x) = \sum_\sigma \frac{N_\sigma}{L} = \frac{N}{L}\,. \tag{5.13}$$

Thus, the density is homogeneous, time-independent, and independent of our choice for the boundary conditions associated with odd and even particle numbers, respectively. To compute the density-density correlation function in the non-interacting limit, we use Eq. (3.28) to obtain

$$G^{(2)}_{\lambda=0,\sigma}(\tau_1,x_1,\tau_2,x_2) = \frac{1}{L}\sum_{k,l} \mathrm{e}^{-|\varepsilon_k^{(I_\sigma)}-\varepsilon_l^{(I_\sigma)}||\tau_1-\tau_2|}\,\theta(\bar{\varepsilon}^{(I_\sigma)}_{\sigma,k})\theta(-\bar{\varepsilon}^{(I_\sigma)}_{\sigma,l})(\phi^{(\mathrm{P})}_{k-l}(x_1))^*\phi^{(\mathrm{P})}_{k-l}(x_2)\,. \tag{5.14}$$

As stated above, the density-density correlation function depends only on $|\tau_1-\tau_2|$. We emphasize again that the density-density correlation function obeys periodic boundary conditions in the spatial direction, independent of our choice for the boundary conditions of the one-particle states, $I_\sigma \in \{P,A\}$. This also holds for the interacting system and can be traced back to the fact that $(\phi_k^{(I)}(x))^*\phi_l^{(I)}(x) \sim \phi^{(\mathrm{P})}_{k-l}(x)$. Moreover, we observe that the density-density correlation function depends only on $|x_1-x_2|$. For the interacting system, however, this is only the case if the interaction potential also exhibits translation invariance. For $\tau_1=\tau_2$, we can rewrite $G^{(2)}_{\lambda=0,\sigma}$ as follows:

$$G^{(2)}_{\lambda=0,\sigma}(0,x_1,0,x_2) = \delta(x_1-x_2)\,n_{\mathrm{gs},\lambda=0,\sigma}(x_1) - \frac{1}{L}\sum_{k,l}\theta(-\bar{\varepsilon}^{(I_\sigma)}_{\sigma,k})\theta(-\bar{\varepsilon}^{(I_\sigma)}_{\sigma,l})(\phi^{(\mathrm{P})}_{k-l}(x_1))^*\phi^{(\mathrm{P})}_{k-l}(x_2)\,, \tag{5.15}$$

where we have used $x_i \in [-L/2, L/2)$ and set $\tau_1=\tau_2=0$ without loss of generality. As it should be, these results for the density-density correlation function are in agreement with our general considerations in Sec. 3.2. In particular, we have

$$\int_{x_1}\int_{x_2} G^{(2)}_{\lambda=0,\sigma}(0,x_1,0,x_2) = 0 \tag{5.16}$$

for any fermion number. For the Fourier transformation of the density-density correlation function we find for $x_1=x_2=0$

$$\tilde{G}^{(2)}_{\lambda=0,\sigma}(\omega,x_1,x_2) = \frac{2}{L}\sum_{k,l}\frac{|\varepsilon_k^{(I_\sigma)}-\varepsilon_l^{(I_\sigma)}|}{\omega^2+|\varepsilon_k^{(I_\sigma)}-\varepsilon_l^{(I_\sigma)}|^2}\,\theta(-\bar{\varepsilon}^{(I_\sigma)}_{\sigma,k})\theta(-\bar{\varepsilon}^{(I_\sigma)}_{\sigma,l})(\phi^{(\mathrm{P})}_{k-l}(x_1))^*\phi^{(\mathrm{P})}_{k-l}(x_2)\,. \tag{5.17}$$

As an example, we also give the initial condition for the total square of the wavefunction for systems of two particles. We distinguish between two cases, a system of two identical particles and a system of two fermions with different spins. In the first case of two identical fermions using Eq. (3.51), we find

$$|\Psi_{\mathrm{gs},\lambda=0}(x_1,x_2)|^2 = \frac{1}{4}\left(\frac{2}{L}\right)^2\left(1-\cos\left(\frac{2\pi(x_1-x_2)}{L}\right)\right) \quad\text{and}\quad |\varphi_{2,\lambda=0}(r)|^2 = \left(\frac{2}{L}\right)^2(L-r)\sin^2\left(\frac{\pi r}{L}\right) \tag{5.18}$$

and for two particles of different spin we find using Eq. (3.52)

$$|\Psi_{\mathrm{gs},\lambda=0}(x_1,x_2)|^2 = \frac{1}{L^2} \quad\text{and}\quad |\varphi_{2,\lambda=0}(r)|^2 = \frac{2(L-r)}{L^2}\,, \tag{5.19}$$

for the absolute square of the ground-state wavefunction and the intrinsic density with $r=|x_1-x_2|\le L$, respectively.

Now that we have introduced the boundary conditions and the corresponding one-particle states and the periodically extended potential we want to revisit the flow equations introduced in Sec. 3.3.

Starting with the flow equation for the density (3.72) we deduce that it is possible to show that the last term vanishes. Using the Fourier-series representation of the potential (5.5) and the fact that we assume the matrix $\mathfrak{U}_{m,n}$ to be diagonal, see Eq. (5.6), we find

$$\int_{x_1}\int_{x_2} U_{\sigma_1\sigma_2}(x_1-x_2)\,\delta(x_2-x_1)\,G^{(2)}_{\lambda,\sigma_1\sigma}(\tau_1,x_1,0,x) = \sum_m \mathfrak{U}^{m,m}_{\sigma_1\sigma_2}\int_{x_1} G^{(2)}_{\lambda,\sigma_1\sigma}(\tau_1,x_1,0,x) = 0\,, \tag{5.20}$$

where we used Eq. (3.63) in the last step. We also observe that this argument holds for all n-density correlation functions $G^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$. Therefore, the flow equation for the density simplifies:

$$\begin{aligned}\partial_\lambda n_{\mathrm{gs},\lambda,\sigma}(x) = &-\sum_{\sigma_1\sigma_2}\int_{\tau_1}\int_{x_1}\int_{x_2} n_{\mathrm{gs},\lambda,\sigma_1}(x_1)\,U_{\sigma_1\sigma_2}(x_1-x_2)\,G^{(2)}_{\lambda,\sigma_2\sigma}(\tau_1,x_2,0,x)\\ &-\frac{1}{2}\sum_{\sigma_1\sigma_2}\int_{\tau_1}\int_{x_1}\int_{x_2} U_{\sigma_1\sigma_2}(x_1-x_2)\,G^{(3)}_{\lambda,\sigma_1\sigma_2\sigma}(\tau_1,x_2,\tau_1,x_1,0,x)\,.\end{aligned} \tag{5.21}$$

We now want to take a deeper look into this flow equation. Therefore we consider the perturbative expansion of the density. We obtain the first-order perturbative correction by plugging the initial conditions for the density (5.13), the density-density correlator (5.14) and the three-density correlator (3.31) into the flow equation (5.21). We find that the right-hand side of the latter equation vanishes:

$$\partial_\lambda n^{(1)}_{\mathrm{gs},\lambda,\sigma}(x) = 0\,. \tag{5.22}$$

This means that the density remains homogeneous at leading-order in the perturbative expansion. In fact, with our choice for the boundary conditions, it follows from the definition of the density as the one-density correlation function, $n_{\mathrm{gs},\lambda,\sigma}(x) = \langle\psi^\dagger_\sigma(x)\psi_\sigma(x)\rangle_\lambda$, that $n_{\mathrm{gs},\lambda,\sigma}$ is homogeneous for any value of λ, i. e. at any order of the perturbative expansion, at least if the ground state is not degenerate:

$$n_{\mathrm{gs},\lambda,\sigma}(x) \equiv n_{\mathrm{gs},\lambda=0,\sigma}(x) = \frac{N_\sigma}{L}\,. \tag{5.23}$$

From this follows that all expansion coefficients $n^{(j)}_{\mathrm{gs},\lambda,\sigma} = 0$ for $j \geq 1$. Thus, we have

$$\partial_\lambda n_{\mathrm{gs},\lambda,\sigma}(x) = 0 \quad \text{for all } \lambda\,. \tag{5.24}$$

As it should be, the leading-order result (5.22) is in accordance with this general statement. We would like to mention that this does by no means imply that the intrinsic density is homogeneous. This is already clear from the result of the non-interacting system with two identical fermions, see Eq. (5.18).

We now come to the flow equation for the density-density correlation function. Using Eq. (5.23) and the analog of Eq. (5.20) for the three-density correlator, the flow equation for $G^{(2)}_{\lambda,\sigma_1,\sigma_2}$ simplifies considerably:

$$\begin{aligned}\partial_\lambda G^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1,x_1,\tau_2,x_2) = &-\sum_{\sigma_3\sigma_4}\int_{\tau_3}\int_{x_3}\int_{x_4} G^{(2)}_{\lambda,\sigma_1\sigma_3}(\tau_1,x_1,\tau_3,x_3)\,U_{\sigma_3\sigma_4}(x_3-x_4)\,G^{(2)}_{\lambda,\sigma_4\sigma_2}(\tau_3,x_4,\tau_2,x_2)\\ &-\frac{1}{2}\sum_{\sigma_3\sigma_4}\int_{\tau_3}\int_{x_3}\int_{x_4} U_{\sigma_3\sigma_4}(x_3-x_4)\,G^{(4)}_{\lambda,\sigma_4\sigma_3\sigma_1\sigma_2}(\tau_3,x_4,\tau_3,x_3,\tau_1,x_1,\tau_2,x_2)\,.\end{aligned} \tag{5.25}$$

With the same line of arguments it is possible to show that in the flow equations of all density correlation functions the terms proportional to the density $n_{\mathrm{gs},\sigma}(x)$ and the terms proportional to the delta distribution $\delta(x_1-x_2)$ vanish.

In the following two chapters we will use the flow equations for the energy (3.83) and the density-density correlation function (5.25) and the result for the density (5.23) to study systems of identical fermions, see Chap. 6, and systems of spin-1/2 fermions, see Chap. 7.

6 Identical Fermions in a One-Dimensional Box

In this chapter, we consider identical fermions in a one-dimensional periodic box with extent L. We aim at a study of the formation of selfbound systems of fermions interacting via a non-local interaction which is repulsive at short distances and attractive at long range. The one-dimensional potential we study here was introduced in the context of Monte-Carlo studies [31].

As introduced in Sec. 3.4, we can recover the results of conventional perturbation theory with our DFT-RG formalism. In this chapter we want to calculate the leading-order and next-to-leading-order correction for the energy of the system under consideration for arbitrary particle numbers. Moreover, we show how our formalism is related to the *Hartree-Fock* approximation.

In a next step, we then employ our DFT-RG approach to compute ground-state properties of systems with N identical fermions. Therefore, we specify the flow equations and introduce the truncations we use in our numerical studies. In Sec. 6.5 we show our DFT-RG results.

Since in this chapter we consider systems of N identical fermions interacting via a two-body interaction, we first show that the flow equation for the ground-state energy vanishes identically if the two-body interaction is simply given by a contact interaction $U(x_1-x_2) = g\,\delta(x_1-x_2)$, as it should be. Plugging this potential in the flow equation for the energy given by Eq. (3.83) we find

$$\partial_\lambda E_\lambda = \frac{g}{2}\int_{x_1}\left(n_{\mathrm{gs},\lambda}(x_1)\,n_{\mathrm{gs},\lambda}(x_2) + G^{(2)}_\lambda(0,x_1,0,x_1) - n_{\mathrm{gs},\lambda}(x_1)\,\delta(0)\right). \tag{6.1}$$

Using Eq. (3.48) and remembering that $\Phi_{N,\lambda}(x,x) = 0$ for identical fermions due to *Pauli* blocking, the right-hand side of the energy flow equation indeed vanishes for any value of λ:

$$\partial_\lambda E_\lambda = 0\,. \tag{6.2}$$

Thus, the energy density functional and likewise the ground-state energy do not change under a variation of λ and therefore remain identical to their initial conditions which are given by a system of N non-interacting identical fermions.

6.1 One-Dimensional Model

For explicit calculations with our DFT-RG approach we adopt a "bare" two-body interaction potential U introduced in Ref. [31]. This interaction potential is given by a superposition of two Gaußians with opposite signs to simulate repulsive short-range and attractive long-range nucleon-nucleon interactions:

$$U_{\mathrm{MC}}(x_1-x_2) = \frac{g}{\sigma_1\sqrt{\pi}}\,\mathrm{e}^{-\frac{(x_1-x_2)^2}{\sigma_1^2}} - \frac{g}{\sigma_2\sqrt{\pi}}\,\mathrm{e}^{-\frac{(x_1-x_2)^2}{\sigma_2^2}}, \tag{6.3}$$

where $g > 0$, $\sigma_1 > 0$, and $\sigma_2 > 0$ are constant parameters, see Fig. 6.1 for an illustration. Throughout this work, we set $m = 1$ for the mass of our toy-model nucleons. This implies that energy is measured in units of inverse length squared and g is measured in units of inverse length. The parameters σ_i set the length scale for the short-range repulsion and the range of attraction, respectively. Following Ref. [31], we choose

$$\bar{g} \equiv g L_0 = 2.4 \quad \text{and} \quad \bar{\sigma}_2 \equiv \sigma_2 L_0^{-1} = 4.0\,, \tag{6.4}$$

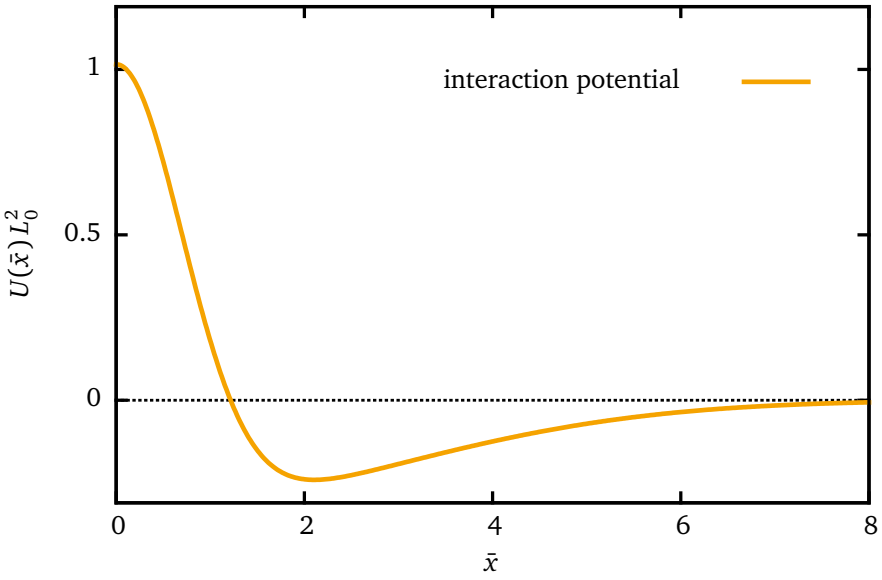

Figure 6.1.: Dimensionless two-body interaction potential $L_0^2 U$ as a function of the dimensionless distance $\bar{x} = x/L_0 := |x_1 - x_2|/L_0$ of two toy-nucleons as determined by the set of parameters given in Eq. (6.4).

where the length scale $L_0 \equiv \sigma_1 = 0.2$ is a measure for the extent of our toy-model nucleons and sets the scale for all dimensionful quantities in our calculations. On the other hand, the parameter σ_2 can be associated with the range of the interaction. In any case, σ_1 and σ_2 are of the same order of magnitude. From a phenomenological point of view, the parameter choice (6.4) ensures that the one-dimensional saturation properties correspond to empirical three-dimensional saturation properties in nuclear physics [31].

Since we consider identical fermions (i. e., fermions with equal spin) in this chapter we omit the spin indices here. The Fourier-series representation of the periodically extended interaction potential U is then given by

$$U(x_1 - x_2) = g \sum_m \mathfrak{U}_{m,m} (\phi_m^{(\mathrm{P})}(x_1))^* \phi_m^{(\mathrm{P})}(x_2)\,. \tag{6.5}$$

6.2 Perturbation Theory

In Sec. 3.4 we showed that we can extract perturbative results within our DFT-RG approach. To this end, we expand the observables, such as the ground-state energy, in powers of some (small) dimensionless parameter $\bar{g}_N$, where the subscript N indicates that this parameter is suitably normalized with the total particle number.

For N fermions in a box with extent L and (anti)periodic boundary conditions the ground-state density $n_{\mathrm{gs},\lambda} = N/L$ is homogeneous for any value of λ. Therefore, we define

$$\bar{g}_N = \frac{gL}{N} \tag{6.6}$$

as the dimensionless coupling parameter.[1]

[1] This definition is common in studies of one-dimensional ultracold gases interacting via a contact interaction [66, 67, 68]. Note that other finite (length) scales enter our calculations. For example, we have finite length scales defining the range of the interaction and the extent of the repulsive core. Thus, the coupling g as a naive measure of the potential energy and the density as a naive measure of the kinetic energy are not the only scales in our numerical studies below. Here, we only use this definition for convenience to define an expansion of the density functional.

The zeroth order of the perturbative expansions of the energy, density and the density correlation functions are given by their initial conditions

$$E_{\mathrm{gs}}^{(0)} \equiv \frac{1}{N} E_{\mathrm{gs},\lambda=0}, \quad n_{\mathrm{gs}}^{(0)} \equiv n_{\mathrm{gs},\lambda=0} \quad \text{and} \quad G^{(2,0)} \equiv G^{(2)}_{\lambda=0}, \tag{6.7}$$

see Sec. 5.2 for explicit expressions.

Using Eq. (3.83) we observe that the computation of the first-order perturbative correction for the ground-state energy only requires the density and density-density correlation function in their zeroth-order approximations, $n_{\mathrm{gs}}^{(0)}$ and $G^{(2,0)}$, respectively. Thus, we have

$$\begin{aligned}\partial_\lambda E_\lambda^{(1)} =& \frac{1}{2L} \int_{x_1} \int_{x_2} n_{\mathrm{gs}}^{(0)}(x_1)\, \mathfrak{U}(x_1 - x_2)\, n_{\mathrm{gs}}^{(0)}(x_2) \\ &+ \frac{1}{2L} \int_{x_1} \int_{x_2} \mathfrak{U}(x_1 - x_2) \Big(G^{(2,0)}(0, x_2, 0, x_1) - n_{\mathrm{gs}}^{(0)}(x_2)\, \delta(x_2 - x_1) \Big) .\end{aligned} \tag{6.8}$$

Note that the general structure of this equation does not depend on the confining geometry. For fermions in a box with (anti)periodic boundary conditions, we obtain

$$E_{\lambda=1}^{(1)} = \int_0^{\lambda=1} \mathrm{d}\lambda' \partial_{\lambda'} E_{\lambda'}^{(1)} = \frac{1}{2} \mathfrak{U}_{0,0} \left(\frac{N}{L} \right)^2 - \frac{1}{2L^2} \sum_{k,l} \theta(-\bar{\varepsilon}_k^{(I)}) \theta(-\bar{\varepsilon}_l^{(I)})\, \mathfrak{U}_{k-l,k-l} . \tag{6.9}$$

Here, we have used Eqs. (5.13) and (5.15).

Now we turn to the computation of the next-to-leading-order correction of the ground-state energy $E_{\mathrm{gs}}^{(2)}$. Plugging the expansions (3.80), (3.81) and (3.82) into flow equation (3.83), we observe that the first-order corrections of the density and the density-density correlation function are needed to calculate $E_{\mathrm{gs}}^{(2)}$.

Since the ground-state density in the interacting case is equal to the initial condition, see Eq. (5.23), all expansion coefficients $n_{\mathrm{gs},\lambda}^{(j)} = 0$ for $j \geq 1$. Therefore, the density term in the flow equation for $E_{\mathrm{gs}}^{(2)}$ vanishes.

To obtain the first-order perturbative correction of the density-density correlation function we have to replace the full correlation functions in Eq. (5.25) by their initial conditions, i. e. $G_\lambda^{(2)} \to G_{\lambda=0}^{(2)} \equiv G^{(2,0)}$ and $G_\lambda^{(4)} \to G_{\lambda=0}^{(4)} \equiv G^{(4,0)}$. The flow equation for $G_\lambda^{(2,1)}$ then reads:

$$\begin{aligned}\partial_\lambda G_\lambda^{(2,1)}(\tau_1, x_1, \tau_2, x_2) =& - \int_{\tau_3} \int_{x_3} \int_{x_4} G^{(2,0)}(\tau_1, x_1, \tau_3, x_3)\, \mathfrak{U}(x_3 - x_4)\, G^{(2,0)}(\tau_3, x_4, \tau_2, x_2) \\ &- \frac{1}{2} \int_{\tau_3} \int_{x_3} \int_{x_4} \mathfrak{U}(x_3 - x_4)\, G^{(4,0)}(\tau_3, x_4, \tau_3, x_3, \tau_1, x_1, \tau_2, x_2) .\end{aligned} \tag{6.10}$$

For the leading-order correction $G_\lambda^{(2,1)}$, we then find[2]

$$\begin{aligned}&G_\lambda^{(2,1)}(\tau_1, x_1, 0, x_2) \\ &\quad = -\lambda \frac{N}{L^3} \sum_{m \neq 0} \mathfrak{U}_{m,m} (\phi_m^{(\mathrm{P})}(x_1))^* \phi_m^{(\mathrm{P})}(x_2) \Bigg\{ \Bigg(\sum_k \theta(-\bar{\varepsilon}_k^{(I)}) \theta(\bar{\varepsilon}_{k+m}^{(I)}) |\tau_1| \mathrm{e}^{-|\varepsilon_{k+m}^{(I)} - \varepsilon_k^{(I)}||\tau_1|} \\ &\qquad - 2 \sum_{k \neq l} \frac{1}{\varepsilon_{k+m}^{(I)} - \varepsilon_{l+m}^{(I)} + \varepsilon_l^{(I)} - \varepsilon_k^{(I)}} \theta(\bar{\varepsilon}_{k+m}^{(I)}) \theta(-\bar{\varepsilon}_k^{(I)}) \Big(\theta(-\varepsilon_l^{(I)}) - \theta(-\varepsilon_{l+m}^{(I)}) \Big) \mathrm{e}^{-|\varepsilon_{k+m}^{(I)} - \varepsilon_k^{(I)}||\tau_1|} \Bigg\} \\ &\qquad + \lambda \frac{N}{L^3} \sum_{k,l} (\phi_{k-l}^{(\mathrm{P})}(x_1))^* \phi_{k-l}^{(\mathrm{P})}(x_2) \Bigg\{ \sum_{m \neq 0} \mathfrak{U}_{m,m} \theta(-\bar{\varepsilon}_k^{(I)}) \Big(\theta(-\bar{\varepsilon}_{l+m}^{(I)}) - \theta(-\bar{\varepsilon}_{k+m}^{(I)}) \Big) |\tau_1| \mathrm{e}^{-|\varepsilon_{k+m}^{(I)} - \varepsilon_{l+m}^{(I)}||\tau_1|} \\ &\qquad + 2 \sum_{m \neq 0} \mathfrak{U}_{m,m} \frac{1}{\varepsilon_{k+m}^{(I)} - \varepsilon_{l+m}^{(I)} + \varepsilon_l^{(I)} - \varepsilon_k^{(I)}} \theta(-\bar{\varepsilon}_k^{(I)}) \theta(\bar{\varepsilon}_l^{(I)}) \Big(\theta(-\bar{\varepsilon}_{l+m}^{(I)}) - \theta(-\bar{\varepsilon}_{k+m}^{(I)}) \Big) \mathrm{e}^{-|\varepsilon_k^{(I)} - \varepsilon_l^{(I)}||\tau_1|} \Bigg\},\end{aligned} \tag{6.11}$$

[2] See Appendix B.1 for a detailed calculation of $G_\lambda^{(2,1)}$.

where we have set $\tau_2 = 0$ for convenience.

Let us now turn to the second order of the perturbative expansion. Using Eq. (3.83) together with the expansions (3.80), (3.81) and (3.82), we find the following expression for the second-order correction to the ground-state energy:

$$\partial_\lambda E^{(2)}_{\mathrm{gs},\lambda} = \frac{1}{L}\int_{x_1}\int_{x_2} \mathfrak{U}(x_1 - x_2)\, G^{(2,1)}_\lambda(0, x_1, 0, x_2)\,. \tag{6.12}$$

Together with Eq. (6.11), we eventually obtain

$$\begin{aligned} E^{(2)}_{\mathrm{gs},\lambda=1} &= \int_0^{\lambda=1} \mathrm{d}\lambda'\, \partial_{\lambda'} E^{(2)}_{\mathrm{gs},\lambda'} \\ &= \frac{1}{L^3}\left(\frac{N}{L}\right) \sum_{m\neq 0}\sum_{k\neq l} \frac{\mathfrak{U}_{m,m}\left(\mathfrak{U}_{k-l,k-l} - \mathfrak{U}_{m,m}\right)}{\varepsilon^{(I)}_{k+m} - \varepsilon^{(I)}_{l+m} - \varepsilon^{(I)}_k + \varepsilon^{(I)}_l}\, \theta(\bar{\varepsilon}^{(I)}_{k+m})\theta(-\bar{\varepsilon}^{(I)}_k)\theta(\bar{\varepsilon}^{(I)}_l)\theta(-\bar{\varepsilon}^{(I)}_{l+m}). \end{aligned} \tag{6.13}$$

We emphasize that this result holds for any particle number N. For $N = 2$ and $N = 3$, we have checked numerically for the interaction potential (6.3) that the results from Eq. (6.13) agree identically with those from conventional second-order perturbation theory.

For $N = 2$, we can calculate the perturbative corrections for the absolute square of the ground-state wavefunction from the expansion coefficients $G^{(2,n)}_\lambda(0, x_1, 0, x_2)$ at order $\bar{g}^n_N$. From Eq. (3.51) we deduce

$$|\Psi^{(n)}_{\mathrm{gs},\lambda}(x_1, x_2)|^2 = \frac{1}{2}\, G^{(2,n)}_\lambda(0, x_1, 0, x_2)\,. \tag{6.14}$$

Note that $G^{(2,1)}_\lambda(0, x_1, 0, x_2) = 0$ for $x_1 = x_2$, in agreement with the *Pauli* principle.

The reconstruction of the perturbative series from our DFT-RG approach can be systematically continued to higher orders in the dimensionless coupling parameter $\bar{g}_N$. For example, to obtain the third-order correction of the energy, we need to insert the second-order correction of the density-density correlation function into the flow equation for the energy which, in turn, requires the computation of the density-density as well as the four-density correlation function at leading order.

6.3 Hartree-Fock Approximation

We would now like to discuss the relation of our approach to the *Hartree-Fock* approximation. This approximation describes the regime where the mean interparticle distance is smaller than the range of the interaction. This approximation is expected to become reliable in the thermodynamic limit ($N/L = $ const. and $L \to \infty$), at least for purely attractive interactions between identical fermions [69, 70, 27]. In this chapter, the interaction under consideration is short-range repulsive and long-range attractive. Thus, the results obtained by the *Hartree-Fock* approximation may only give good results in a certain density range where the mean interparticle distance is of the order of the interaction range but still sufficiently larger than the scale associated with the short-range repulsion. For the two-body potential (6.3) such a density regime may be small if it exists at all. From a field-theoretical point of view a study of the relation between the *Hartree-Fock* approximation and our DFT-RG approach will nevertheless be instructive. We consider Eq. (6.8), which yields the leading-order correction to the ground-state energy, and use Eqs. (5.7) and (5.15) to obtain:

$$\begin{aligned} \frac{1}{N} E^{\mathrm{LO}}_{\lambda=1} =& \frac{1}{N}\sum_n \varepsilon^{(I)}_n \theta(-\bar{\varepsilon}^{(I)}_n) + \frac{g}{2N}\sum_{k,l}\theta(-\bar{\varepsilon}^{(I)}_k)\theta(-\bar{\varepsilon}^{(I)}_l)\int_{x_1}\int_{x_2} (\phi^{(I)}_k(x_1))^* \phi^{(I)}_k(x_1)\mathfrak{U}(x_1 - x_2)(\phi^{(I)}_l(x_2))^* \phi^{(I)}_l(x_2) \\ &- \frac{g}{2N}\sum_{k,l}\theta(-\bar{\varepsilon}^{(I)}_k)\theta(-\bar{\varepsilon}^{(I)}_l)\int_{x_1}\int_{x_2} \mathfrak{U}(x_1 - x_2)(\phi^{(I)}_k(x_1))^*(\phi^{(I)}_l(x_2))^* \phi^{(I)}_l(x_1)\phi^{(I)}_k(x_2)\,, \end{aligned} \tag{6.15}$$

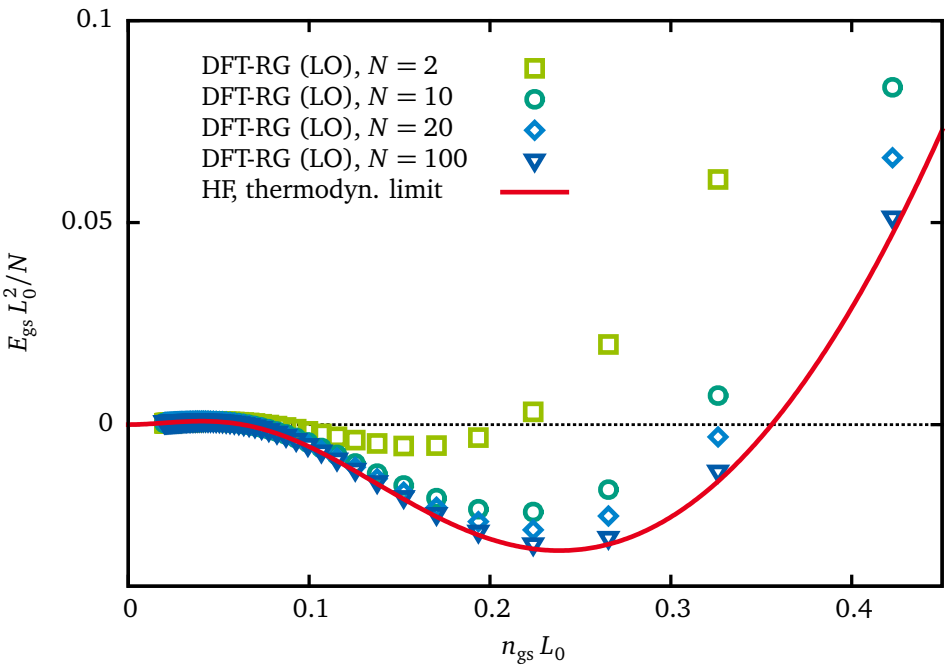

Figure 6.2.: Energy per fermion E/N for $N = 2, 10, 20, 100$ fermions as a function of $n_{gs} = N/L$ as obtained from our DFT-RG approach at leading order (LO), see Eq. (6.15). Here, L is measured in units of L_0. For fixed $n_{gs} = N/L$, the leading-order DFT-RG results approach the Hartree-Fock (HF) approximation of the equation of state in the limit $N \to \infty$, see Eq. (6.19).

where we have used that

$$n_{gs,\lambda}(x) = \sum_k \theta(-\bar{\varepsilon}_k^{(I)})(\phi_k^{(I)}(x))^* \phi_k^{(I)}(x). \tag{6.16}$$

The first term on the right-hand side of Eq. (6.15) is associated with the kinetic energy of the fermions. The second term is the so-called *Hartree* term and the third term is the so-called exchange or *Fock* term. The expression (6.15) can be identified with the *Hartree-Fock* energy as obtained from a *Slater* determinant defined by one-particle wavefunctions $\phi_n^{(I)}$. We shall refer to Eq. (6.15) as the leading-order (LO) DFT-RG approximation.[3]

This leading-order approximation can also be obtained by setting $\partial_\lambda G_\lambda^{(n)} = 0$ for $n \geq 1$. This does not imply that $G_\lambda^{(n)} = 0$ for $n \geq 1$, but rather that the density correlation functions remain at their initial conditions. Since we obtained the leading-order perturbative correction by plugging the initial condition $G_{\lambda=0}^{(2)}$ into the flow equation for the energy, it is immediately clear that our leading-order DFT-RG approximation is identical to the leading-order perturbative approximation, see our discussion in Sec. 6.2. We therefore conclude that the *Hartree-Fock* approximation obtained within our DFT-RG approach can be associated with the leading-order correction of the ground-state energy in an expansion in powers of the small coupling parameter $\bar{g}_N$.

In Fig. 6.2, we show $E/N \equiv E_{\lambda=1}^{\mathrm{LO}}/N$ for $N = 2, 10, 20, 100$ as a function of the ground-state density n_{gs} as obtained from Eq. (6.15).

The *Hartree-Fock* approximation of the equation of state can be obtained from Eq. (6.15) by taking the thermodynamic limit. In this limit, the momenta p of the fermions become continuous and the associated one-particle wavefunctions are given by

$$\phi_p(x) = \frac{1}{\sqrt{L}} \mathrm{e}^{-\mathrm{i}px}, \tag{6.17}$$

[3] Note that Eq. (6.15) is a *universal* result in the sense of being independent of the choice of the regulator function $\mathcal{R}_\lambda$ implicitly introduced in Eq. (3.1). This follows immediately from the general properties of $\mathcal{R}_\lambda$ specified in Eq. (3.2).

where the volume-dependent prefactor normalizes these states and the limit $L \to \infty$ is assumed to be taken in the end. The Fourier transform $\mathfrak{U}(p)$ of the function $\mathfrak{U}(x_1 - x_2)$ is then defined as follows:

$$\mathfrak{U}(x_1 - x_2) = \sum_m \mathfrak{U}_{m,m} (\phi_m^{(\mathrm{P})}(x_1))^* \phi_m^{(\mathrm{P})}(x_2) \overset{(L\to\infty)}{\longrightarrow} \int_{-\infty}^{\infty} \frac{\mathrm{d}p}{2\pi} \mathfrak{U}(p) \mathrm{e}^{\mathrm{i}p(x_1 - x_2)}, \tag{6.18}$$

where $\mathfrak{U}_{m,m}$ and $\mathfrak{U}(p)$ are both dimensionless. With these conventions defined, it is now possible to obtain the *Hartree-Fock* energy E_{HF} in the thermodynamic limit from Eq. (6.15). In agreement with the literature [27], we find

$$\frac{1}{N} E_{\mathrm{HF}} = \frac{k_{\mathrm{F}}^2}{6} + \frac{\bar{g}_N}{2} \int_{-k_{\mathrm{F}}}^{k_{\mathrm{F}}} \frac{\mathrm{d}p_1}{2\pi} \int_{-k_{\mathrm{F}}}^{k_{\mathrm{F}}} \frac{\mathrm{d}p_2}{2\pi} \left(\mathfrak{U}(0) - \mathfrak{U}(p_1 - p_2) \right), \tag{6.19}$$

where $k_{\mathrm{F}} = \pi N/L$ is the *Fermi* momentum and $\bar{g}_N = gL/N = g\pi/k_{\mathrm{F}}$. Here, the first term is the limit of the kinetic energy term of Eq. (6.15) and the second term is the limit of the *Fock* term. The *Hartree* term vanishes identically for the given two-body potential (6.3) in this termodynamic limit, i. e., $\mathfrak{U}(p) \to 0$ for $p \to 0$. For this very potential holds that for any finite momentum p the Fourier transformation $\mathfrak{U}(p) > 0$ is finite. These are characteristics of the potential under consideration (6.3) and imply, loosely speaking, that in the limit of vanishing momentum transfer fermions do not interact. For small momentum transfers we find $\mathfrak{U}(p) \sim p^2$ for the two-body potential defined in Eq. (6.3). Considering the second term in Eq. (6.19), the *Fock* or exchange term, we find for the limit of small densities, that this term scales as $k_{\mathrm{F}}^3 \sim (N/L)^3$ and is therefore subleading compared to the kinetic energy. This implies that E_{HF}/N approaches zero from above. On the other hand, for large densities we find that the exchange energy becomes constant for $k_{\mathrm{F}} \sim N/L \to \infty$ and is again subleading in comparison with the kinetic energy term.

6.4 DFT-RG Flow Equations

Before we discuss our numerical results, we specify the flow equations underlying our studies. To this end, we make use of the findings from our discussion of the relation between the DFT-RG approach and many-body perturbation theory. Using Eqs. (3.71) and (6.9), we find the following differential equation for the ground-state energy:

$$\frac{1}{N} \partial_\lambda E_\lambda = \frac{\bar{g}_N}{2} \mathfrak{U}_{0,0} \left(\frac{N}{L} \right)^2 - \frac{\bar{g}_N}{2L^2} \sum_{k,l} \theta(-\bar{\varepsilon}_k^{(I)}) \theta(-\bar{\varepsilon}_l^{(I)}) \mathfrak{U}_{k-l,k-l} + \frac{\bar{g}_N}{2L} \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \sum_a \mathfrak{U}_{a,a} \Delta \tilde{G}_{\lambda,a,a}^{(2)}(\omega), \tag{6.20}$$

where we have tacitly introduced the Fourier transform of the density-density correlation function $G_\lambda^{(2)}$,

$$G_\lambda^{(2)}(\tau_1, x_1, \tau_2, x_2) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi} \sum_{a,b} \tilde{G}_{\lambda,a,b}^{(2)}(\omega) (\phi_a^{(\mathrm{P})}(x_1))^* \phi_b^{(\mathrm{P})}(x_2) \mathrm{e}^{-\mathrm{i}\omega(\tau_1 - \tau_2)}. \tag{6.21}$$

In Eq. (6.20), we have decomposed this function into the density-density correlation function of the non-interacting system ($\lambda = 0$) and its modification $\Delta G_\lambda^{(2)}$ in the presence of interactions between the fermions:

$$\tilde{G}_{\lambda,a,b}^{(2)}(\omega) = \tilde{G}_{\lambda=0,a,b}^{(2)}(\omega) + \Delta \tilde{G}_{\lambda,a,b}^{(2)}(\omega). \tag{6.22}$$

This decomposition is convenient from a numerical point of view as it allows us to treat those terms on the right-hand side of the flow equation for $\tilde{G}_{\lambda,a,b}^{(2)}$ analytically which contain contributions of the form $\sim \delta(x_i - x_j)$, see Eq. (6.28) below. In any case, the initial condition for the energy is given by the energy of the non-interacting N-fermion system, see Eq. (5.7).

As discussed in Sec. 5.3, the flow equation of the ground-state density n_{gs} is equal to zero. At this point we would like to emphasize again that the ground-state density n_{gs} should by no means be confused with the intrinsic density

of the system. For the two-body system the latter can be obtained from the density-density correlation function, see Eq. (3.48), and is a non-trivial function. In general, we need the N-density correlation function $G_\lambda^{(N)}$ to compute the intrinsic density of the N-fermion system.

For the density-density correlation function, the exact flow equation reads

$$\begin{aligned}\partial_\lambda G_\lambda^{(2)}(\tau_1,x_1,\tau_2,x_2) = &-\int_{\tau_3}\int_{x_3}\int_{x_4} G_\lambda^{(2)}(\tau_1,x_1,\tau_3,x_3)U(x_3-x_4)G_\lambda^{(2)}(\tau_3,x_4,\tau_2,x_2)\\ &-\frac{1}{2}\int_{\tau_3}\int_{x_3}\int_{x_4} U(x_3-x_4)G_\lambda^{(4)}(\tau_3,x_4,\tau_3,x_3,\tau_1,x_1,\tau_2,x_2)\,. \end{aligned} \tag{6.23}$$

We shall neglect the flow of all correlation functions $G_\lambda^{(n)}$ with $n>2$ in our numerical studies. Note that this does not imply that we set the higher-order correlation functions to zero, it rather means that we replace, e. g., $G_\lambda^{(4)}$ by $G_{\lambda=0}^{(4)}$ in the flow equation of the density-density correlation function. In general, the initial conditions of the n-density correlation functions are also finite. As discussed in Sec. 6.2, we can obtain the first-order perturbative correction of $G_\lambda^{(2)}$ if we replace also the density-density correlation functions appearing on the right-hand side of Eq. (6.23) by their initial conditions. With this we can then obtain the second-order perturbative result for the energy. To go beyond second-order perturbation theory we solve the flow equation (6.23) without replacing $G_\lambda^{(2)}$ by $G_{\lambda=0}^{(2)}$ and thereby take arbitrarly high orders in $\bar{g}_N$ into account. Using Eq. (3.48) to compute the quantity $\Phi_{N,\lambda}(x_1,x_2)$ within this approximation, we find that the latter is finite for $x_1\to x_2$. Thus, this truncation is not consistent with the *Pauli* principle.

If we would solve the flow equation (6.23) with the exact four-density correlation function $G_\lambda^{(4)}$, the result would be in agreement with the *Pauli* exclusion principle. To this end, we would have to solve the complete infinite tower of flow equations, which is impossible. The second possibility is to improve our truncation such that the *Pauli* exclusion principle is respected for any value of λ. The *Pauli* exclusion principle is associated with the condition $\Phi_{N,\lambda}(x,x)=0$ for $\lambda\in[0,1]$, which is equivalent to the condition

$$\Delta G_\lambda^{(2)}(0,x,0,x)=0\,. \tag{6.24}$$

This follows from the decomposition of $G_\lambda^{(2)}$ into $G_{\lambda=0}^{(2)}$ and $\Delta G_\lambda^{(2)}$ together with Eqs. (3.48) and (5.15). For $\lambda=0$, this condition is trivially satisfied. For any finite λ, a sufficient criterion to satisfy this condition is obtained by requiring that the flow of $\Delta G_\lambda^{(2)}$ vanishes identically for $\tau_1=\tau_2=0$ and $x_1=x_2=x$:

$$\partial_\lambda \Delta G_\lambda^{(2)}(0,x,0,x)=0\,. \tag{6.25}$$

Since we would like to retain the truncation scheme introduced above, i. e., we neglect the flow of all correlation functions $G_\lambda^{(n)}$ with $n>2$ and replace the remaining n-density correlation function with $n>2$, namely $G_\lambda^{(4)}$, by its initial condition $G_{\lambda=0}^{(4)}$, we can obtain a simple but non-trivial modification of the flow equation (6.23) that is in agreement with the *Pauli* exclusion principle by replacing

$$G_{\lambda=0}^{(4)}(\chi_1,\chi_2,\chi_3,\chi_4)\to f_{\mathscr{P}}(\lambda)G_{\lambda=0}^{(4)}(\chi_1,\chi_2,\chi_3,\chi_4)\,. \tag{6.26}$$

Here, the "*Pauli*-blocking function" $f_{\mathscr{P}}$ does not depend on the spatial and the time-like coordinates but only on the flow parameter λ. For $\tau_1=\tau_2=0$ and $x_1=x_2=0$,[4] we can obtain the following expression for the function $f_{\mathscr{P}}$ from the flow equation for the density-density correlation function:

$$\begin{aligned} f_{\mathscr{P}}(\lambda) = &-2\left(\int_{\tau_3}\int_{x_3}\int_{x_4} G_\lambda^{(2)}(0,0,\tau_3,x_3)U(x_3-x_4)G_\lambda^{(2)}(\tau_3,x_4,0,0)\right)\\ &\times\left(\int_{\tau_3}\int_{x_3}\int_{x_4} U(x_3-x_4)G_{\lambda=0}^{(4)}(\tau_3,x_4,\tau_3,x_3,0,0,0,0)\right)^{-1}. \end{aligned} \tag{6.27}$$

[4] Without loss of generality, we have set $x_1=x_2=0$ since the density-density correlation function does only depend on $|x_1-x_2|$ in our present study. For other confining geometries and interaction potentials, this prescription yields a function $f_{\mathscr{P}}$ which depends on the spatial coordinates.

For $\lambda \to 0$, we have $f_{\mathscr{P}}(\lambda) \to 1$. Within the present truncation, this follows directly from the fact that the right-hand side of Eq. (6.23) approaches the leading-order result for $G_\lambda^{(2)}$ in the perturbative expansion, see also our discussion in Sec. 6.2. Taking the function $f_{\mathscr{P}}$ into account, we obtain the following flow equations for the Fourier coefficients $\Delta\tilde{G}^{(2)}_{\lambda,a,a}(\omega)$:

$$\partial_\lambda \Delta\tilde{G}^{(2)}_{\lambda,a,a}(\omega) = -g\left(\Delta\tilde{G}^{(2)}_{\lambda,a,a}(\omega)\mathfrak{U}_{a,a}\,\Delta\tilde{G}^{(2)}_{\lambda,a,a}(\omega) + 2\,\tilde{G}^{(2)}_{0,a,a}\,\mathfrak{U}_{a,a}\,\Delta\tilde{G}^{(2)}_{\lambda,a,a}(\omega) + \mathscr{G}^{(2,1)}_{a,a}(\omega) + f_{\mathscr{P}}(\lambda)\,\mathscr{G}^{(4,1)}_{a,a}(\omega)\right), \quad (6.28)$$

where

$$\tilde{G}^{(2)}_{0,a,a}(\omega) = \frac{2}{L}\sum_k \theta(\bar{\varepsilon}^{(I)}_k)\theta(-\bar{\varepsilon}^{(I)}_{k-a})\frac{|\varepsilon^{(I)}_k - \varepsilon^{(I)}_{k-a}|}{\omega^2 + |\varepsilon^{(I)}_k - \varepsilon^{(I)}_{k-a}|^2} \quad (6.29)$$

is the a-th Fourier coefficient of the density-density correlation function of the non-interacting system. The quantities $\mathscr{G}^{(2,1)}_{a,a}$ and $\mathscr{G}^{(4,1)}_{a,a}$ are defined as[5]

$$\begin{aligned}\tilde{\mathscr{G}}^{(2,1)}_{a,a}(\omega) = &\frac{2}{L^2}\,\mathfrak{U}_{a,a}\Bigg\{\sum_k \theta(-\bar{\varepsilon}^{(I)}_k)\theta(\bar{\varepsilon}^{(I)}_{k+a})\frac{|\varepsilon^{(I)}_{k+a} - \varepsilon^{(I)}_k|^2 - \omega^2}{(\omega^2 + |\varepsilon^{(I)}_{k+a} - \varepsilon^{(I)}_k|^2)^2} \\ &- 2\sum_{k\neq l}\frac{1}{\varepsilon^{(I)}_{k+a} - \varepsilon^{(I)}_{l+a} + \varepsilon^{(I)}_l - \varepsilon^{(I)}_k}\theta(\bar{\varepsilon}^{(I)}_{k+a})\theta(-\bar{\varepsilon}^{(I)}_k)\left(\theta(-\varepsilon^{(I)}_l) - \theta(-\varepsilon^{(I)}_{l+a})\right)\frac{|\varepsilon^{(I)}_{k+a} - \varepsilon^{(I)}_k|}{\omega^2 + |\varepsilon^{(I)}_{k+a} - \varepsilon^{(I)}_k|^2}\Bigg\}, \quad (6.30)\\ \tilde{\mathscr{G}}^{(4,1)}_{a,a}(\omega) = &-\frac{2}{L^2}\sum_k\sum_{m\neq 0}\mathfrak{U}_{m,m}\Bigg\{\theta(-\bar{\varepsilon}^{(I)}_k)\left(\theta(-\bar{\varepsilon}^{(I)}_{k-a+m}) - \theta(-\bar{\varepsilon}^{(I)}_{k+m})\right)\frac{|\varepsilon^{(I)}_{k+m} - \varepsilon^{(I)}_{k-a+m}|^2 - \omega^2}{(\omega^2 + |\varepsilon^{(I)}_{k+m} - \varepsilon^{(I)}_{k-a+m}|^2)^2} \\ &+ \frac{2}{\varepsilon^{(I)}_{k+m} - \varepsilon^{(I)}_{k-a+m} + \varepsilon^{(I)}_{k-a} - \varepsilon^{(I)}_k}\theta(-\varepsilon^{(I)}_k)\theta(\varepsilon^{(I)}_{k-a})\left(\theta(-\bar{\varepsilon}^{(I)}_{k-a+m}) - \theta(-\bar{\varepsilon}^{(I)}_{k+m})\right)\frac{|\varepsilon^{(I)}_k - \varepsilon^{(I)}_{k-a}|}{\omega^2 + |\varepsilon^{(I)}_k - \varepsilon^{(I)}_{k-a}|^2}\Bigg\}. \quad (6.31)\end{aligned}$$

The initial condition for the differential equations (6.28) are $\Delta\tilde{G}^{(2)}_{\lambda,a,a}(\omega) = 0$ for $a \in \mathbb{Z}$ and $\omega \in \mathbb{R}$. Note that the function $f_{\mathscr{P}}$ depends implicitly on all coefficients $\Delta\tilde{G}^{(2)}_{\lambda,a,a}(\omega)$. Therefore, the flow equations for these quantities are coupled whereas they are decoupled if we set $f_{\mathscr{P}}(\lambda) = 1$ for $\lambda \in [0,1]$. In the following we refer to the set of equations (6.20) and (6.28) as the next-to-leading-order (NLO) approximation within our DFT-RG framework, as it appears to be the most natural extension of the leading-order approximation which we have introduced and discussed in Sec. 6.3.

For our numerical calculations we have introduced a cutoff Λ_F for the Fourier modes to solve the flow equations (6.20) and (6.28). We checked the convergence of the results as a function of the cutoff. More specifically, we used values for Λ_F up to $\Lambda_\mathrm{F} = 400$ for $N = 10$ in the volume range considered in this work and found that, e. g., the results for the ground-state energy for $N = 10$ for $\Lambda_\mathrm{F} = 300$ and $\Lambda_\mathrm{F} = 400$ only deviate on the sub-per-mille level, provided the cutoff associated with the integrations over ω on the right-hand side of the flow equations has been chosen sufficiently large. To perform the ω integrations numerically we projected the interval $(-\infty, \infty)$ onto the compact interval $[-1, 1]$ using the mapping function

$$\bar{\omega} = \frac{2}{\pi}\arctan\left(s_\omega \omega L^2\right). \quad (6.32)$$

Here, s_ω is a dimensionless scaling factor at our disposal. Standard *Chebyshev-Gauss* quadrature can then be employed to perform the integrations over ω, where s_ω can be used to improve the convergence. We have checked that our results are converged as a function of the cutoff Λ_C for the *Chebyshev* nodes $\bar{\omega}_i$,

$$\bar{\omega}_i = \cos\left(\frac{2i-1}{2\Lambda_\mathrm{C}}\pi\right). \quad (6.33)$$

[5] The quantities $\mathscr{G}^{(2,1)}_{a,a}$ and $\mathscr{G}^{(4,1)}_{a,a}$ are related to the two terms on the right-hand side of the flow equation of $G^{(2,1)}_\lambda$, see Eq. (6.10). The detailed calculation of these two quantities can be found in App. B.1.

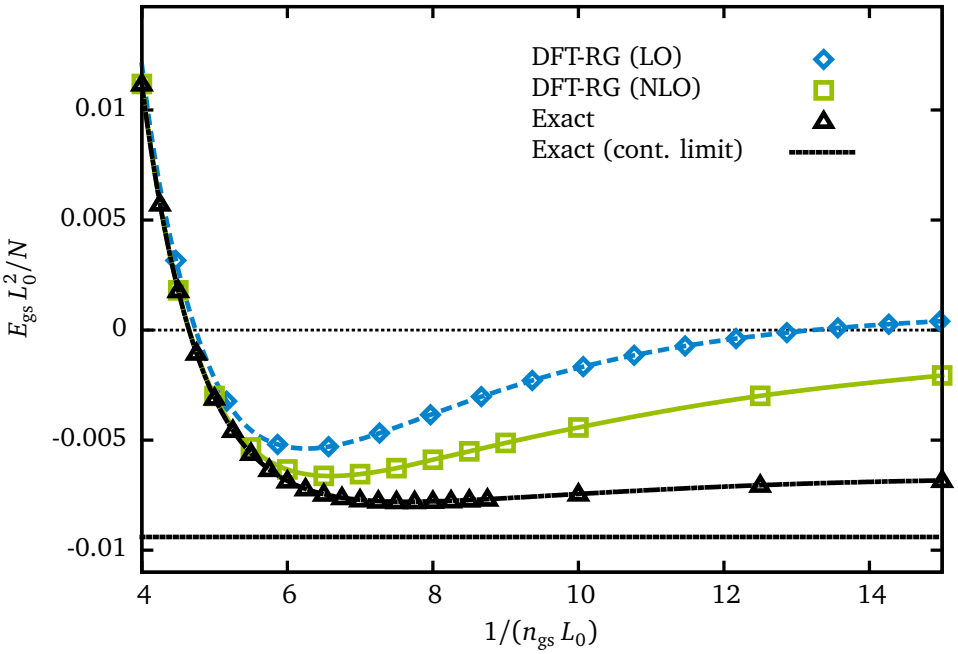

Figure 6.3.: Ground-state energy of the two-body problem as a function of the inverse ground-state density as obtained from different studies. Note that the ground-state density should not be confused with the intrinsic density of the system, see main text for details.

In the numerical studies discussed below, we specifically used values for Λ_C up to $\Lambda_C = 280$ for $N = 10$. These high values are necessary to fulfill the condition (6.24), associated with the *Pauli* principle in the RG flow. This is due to the fact that the latter requires that the tail of the density-density correlation function in the large ω-limit ($\sim 1/\omega^2$) is resolved accurately. In future studies, it could be possible to improve the convergence of our results with respect to Λ_C if one improves the distribution of the *Chebyshev* nodes. This distribution is partially controlled by the function (6.32) that maps the infinit interval for ω on a compact interval. Note that the result for the ground-state energy converges faster as a function of Λ_C.

6.5 DFT-RG Results – Ground-State Properties of Bound States

Let us finally discuss the results from the numerical solution of the DFT-RG flow equations. In Fig. 6.3, we show the ground-state energy per fermion E/N for $N = 2$ as a function of the inverse ground-state density n_{gs} as obtained from different calculations, namely DFT-RG in the leading-order (LO) approximation as given by Eq. (6.15), DFT-RG in the next-to-leading-order (NLO) approximation as discussed in Sec. 6.4, and the exact result as obtained from a diagonalization of the Hamilton operator in a sufficiently large subspace spanned by the two-particle wavefunctions of the non-interacting system in the box. For comparison, we also show the result for the ground-state energy of the two-body problem in the continuum limit which has been calculated by solving the *Schrödinger* equation in the center-of-mass frame in a sufficiently large subspace spanned by harmonic oscillator eigenfunctions. We stress again that $n_{gs} = N/L$ in Fig. 6.3 should by no means be confused with the intrinsic density of the system. For $N = 2$, the latter can be extracted from the density-density correlation function, see Eqs. (3.48) and (3.53) as well as Fig. 6.4.

In Fig. 6.3 we observe that the results for the ground-state energy from our DFT-RG approximation approach the exact solution from above. For small $1/n_{gs} = N/L$, this means for high densities or small box sizes, our DFT-RG results in leading order and next-to-leading order are in very good agreement with the exact result. In particular, for $1/n_{gs} \lesssim 4\,L_0$, our DFT-RG results already agree identically with the exact solution on the scale of the plot. For higher densities, $1/n_{gs} \lesssim 2.9\,L_0$, the energy of the interacting system becomes even larger than the energy

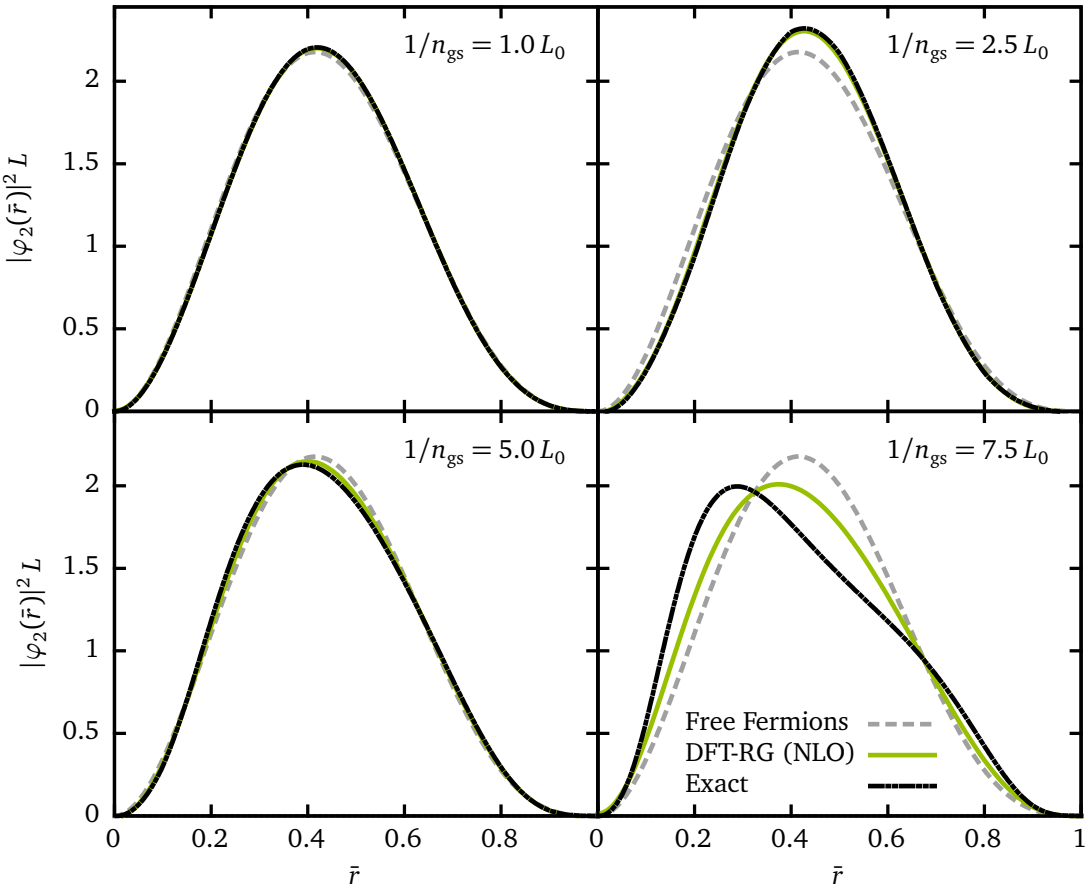

Figure 6.4.: Dimensionless absolute square of the ground-state wavefunction $|\varphi_2(\bar{r})|^2\,L$ in the center-of-mass frame as a function of $\bar{r} = r/L$ as obtained from our DFT-RG approach at NLO in comparison with the exact solution and the result for the non-interacting two-body system.

of the non-interacting two-body system. This is due to the fact that the interaction under consideration has a repulsive core and for small box sizes the latter gives the dominant contribution to the energy, while the long-range attractive tail of the interaction is cut off. Therefore the high energies for small volumes come not only from the increase of the kinetic energy $\sim 1/L^2$ but also from the repulsive core of the underlying interaction. For large volumes $1/n_{gs} \gtrsim 4\,L_0$ the results from our leading-order DFT-RG approximation start to deviate from the next-to-leading-order results and the exact solution. For $1/n_{gs} \gtrsim 6\,L_0$, we find that also the next-to-leading-order DFT-RG result deviates significantly from the exact solution.

The results from both our DFT-RG approximations for the energy per particle assume a minimum at a vinite value of $1/n_{gs}$, whereas the exact result appears to "flatten out" already around $1/n_{gs} \sim 6\,L_0$. Moreover, the exact solution approaches a finite value in the continuum limit, i. e., for $1/n_{gs} \to \infty$. We conclude that our present truncation is not able to reproduce the exact scaling behavior of the density-density correlation functions for large volumes which is important to recover the exact result in the continuum-limit. In the low-density regime the contributions from higher-order density correlation functions are important and we cannot neglect their flows anymore.

In addition, we can observe in Fig. 6.3 that the exact solution for the ground-state energy in the finite box approaches the continuum-limit value from above. We will use this observation below. Note that the exact solution assumes a local maximum $E/N \approx -0.0068\,(1/L_0^2)$ at $1/n_{gs} \approx 17.5\,L_0$, decreases again for larger volumes and converges slowly to the continuum-limit result $E/N|_{\text{cont.}} \approx -0.0094\,(1/L_0^2)$. In fact, for $1/n_{gs} \approx 80\,L_0$, the exact solution in the box still deviates from the continuum-limit result by $\sim 10\%$. This slow convergence may indicate that the low-momentum modes that are cut off in the presence of the finite box are important to obtain an accurate description of the dynamics in the continuum limit.

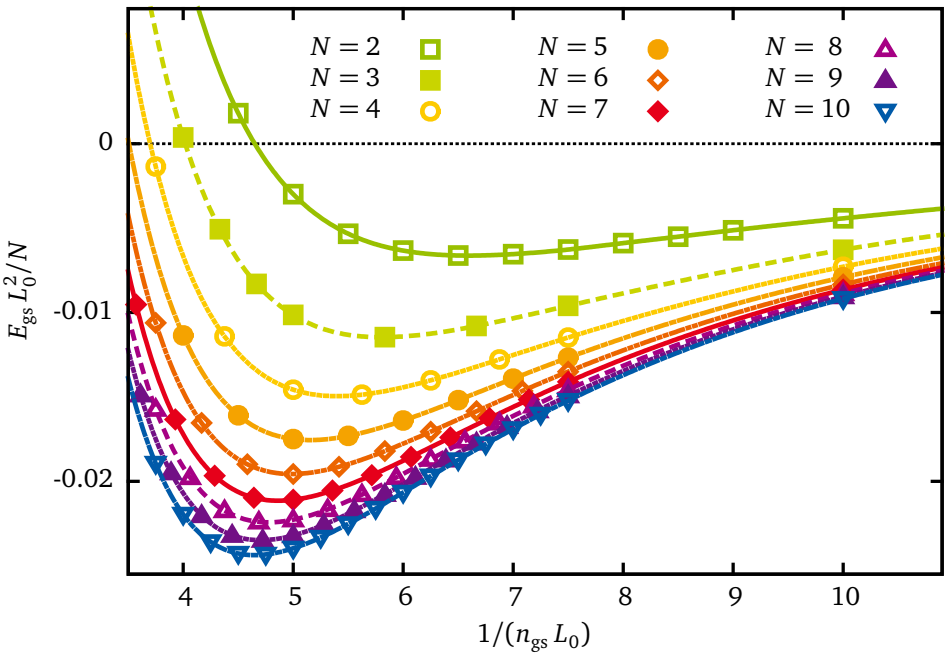

Figure 6.5.: Ground-state energy of various N-fermion systems as a function of the inverse ground-state density. Note that the latter should not be confused with the intrinsic density of the system, see main text for details.

Now we would like to make a comment about the center-of-mass energy. It is possible to decompose the total energy E into the binding energy E_B and the center-of-mass energy E_{cm} associated with the free motion of the center of mass of the N-fermion system, $E = E_{cm} + E_B$. For fermions in a box with (anti)periodic boundary conditions the center-of-mass energy vanishes and the total energy is given by the binding energy, $E = E_B$. This holds for any number of fermions and therefore we conclude that our results for the energy are not spoilt by contributions associated with the center-of-mass motion of the system.

Additionally, we briefly discuss the spourios fermion self-interactions mentioned above. The ground-state energy of a system with a single fermion is zero in a box with periodic boundary conditions. In Sec. 3.7 we have proven that the ground-state energy also vanishes in our DFT-RG framework, if we solve the infinite set of flow equations. For any truncation this may not be the case and we expect that our results for the ground-state energy could be contaminated by contributions from spurious self-interactions. To test the quality of our DFT-RG result in next-to-leading order, we have computed the ground-state energy also for a single fermion. We find that $EL_0^2 \lesssim \mathcal{O}(10^{-4})$ for $1/(n_{gs}L_0) \gtrsim 6$ which is about 1% of the exact result for the ground-state energy of the two-body problem in this range.[6] We find this value for EL_0^2 for $N = 1$ reasonably small, as it is obtained by the simplest truncation containing the flow equation of the density-density correlation function.

We now come to the discussion of our results for the absolute square of the ground-state wavefunction $|\varphi_2(\bar{r})|^2$ in the center-of-mass frame, i. e. the so-called intrinsic density. These results can be extracted from the density-density correlation function, see Eqs. (3.48) and (3.53). In Fig. 6.4, we show the result for the dimensionless intrinsic density $|\varphi_2(\bar{r})|^2 L$ as a function of $\bar{r} = r/L = |x_1 - x_2|/L$ as obtained from our next-to-leading-order DFT-RG study, in comparison with the exact solution and the result for the non-interacting system. As a consequence of the use of antiperiodic boundary conditions, in the case of $N = 2$ the ground-state density n_{gs} is constant, whereas the intrinsic density of the two-body body system develops a non-trivial dependence on the spatial coordinate. For the non-interacting system the dimensionless quantity $|\varphi_2(\bar{r})|^2 L$ as a function of $\bar{r}$ is universal, i. e., independent of the ground-state density n_{gs}. In contrast to this we observe that the exact solution as well as our DFT-RG results

[6] At leading order, E/N vanishes identically for $N = 1$ within our DFT-RG framework.

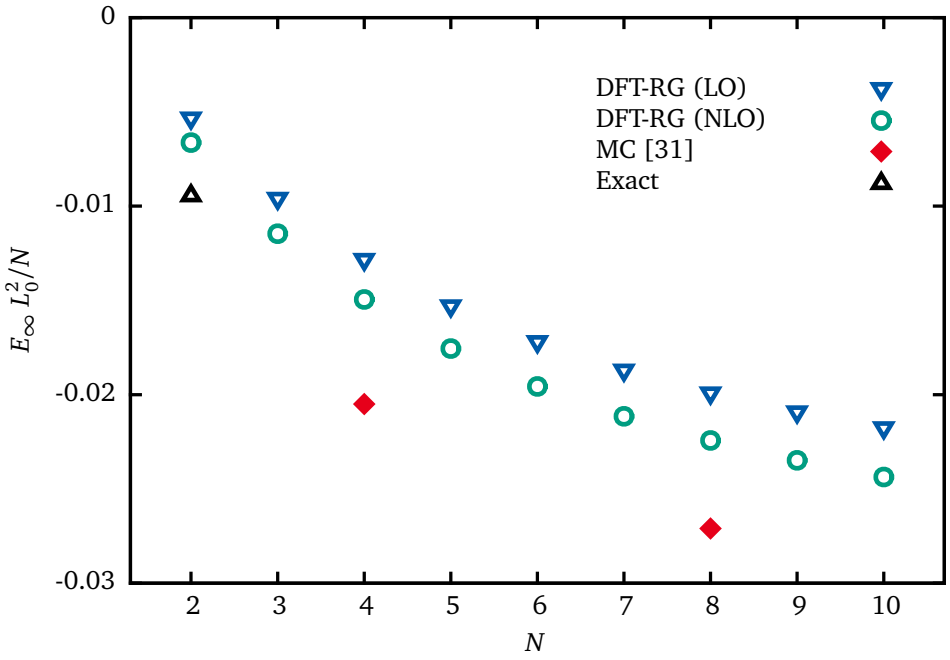

Figure 6.6.: Estimates for the ground-state energy per fermion E/N for systems with $N = 2, \ldots, 10$ fermions in the continuum limit compared to the exact result for $N = 2$ and MC results [31] for $N = 4$ and $N = 8$. Note that an MC result for $N = 2$ in the continuum limit is not given in Ref. [31] but only for the finite-volume case which we find to be in disagreement with our exact solution. For $N = 4$ and $N = 8$, the MC results for the infinite-volume limit are found to be in good agreement with Hartree-Fock calculations in the infinite-volume limit [31].

depend on n_{gs}. In particular, for $1/n_{\mathrm{gs}} \gtrsim 5\,L_0$, we find that the maximum of $|\varphi_2(\bar{r})|^2 L$ is shifted to smaller values of the dimensionless quantity $\bar{r}$ for increasing box sizes. For sufficiently large volumes, the exact solution $|\varphi_2(\bar{r})|^2$ in a finite box then approaches the solution in the continuum limit. In particular for the maximum of $|\varphi_2(\bar{r})|^2 L$, we have $\bar{r}_{\mathrm{max}}(L) \sim r_{\mathrm{max}}(\infty)/L$ for the exact solution, where the constant $r_{\mathrm{max}}(\infty) > 0$ is the position of the maximum in the continuum limit and roughly coincides with the position of the minimum of the interaction potential, see Fig. 6.1. In accordance with our discussion of the ground-state energy, we observe that our DFT-RG results for $|\varphi_2(\bar{r})|^2$ are in very good agreement with the exact solution for $1/n_{\mathrm{gs}} \lesssim 5\,L_0$. For $1/n_{\mathrm{gs}} \gtrsim 5\,L_0$, our DFT-RG results then start to deviate from the exact solution. For $1/n_{\mathrm{gs}} = 7.5\,L_0$, we already find a significant difference between our DFT-RG result at next-to-leading order and the exact result. Since the intrinsic density is extracted from the density-density-correlation function, we conclude that this quantity also differs significantly from the exact result, which enters into the results of the ground-state energy, see Fig. 6.3.

Now we come finally to the discussion of systems with higher fermion numbers. In Fig. 6.5, we show our results for the ground-state energy per fermion E/N as a function of the inverse ground-state density $1/n_{\mathrm{gs}}$ for $N = 2, 3, \ldots, 10$ fermions. We observe that the results for different fermion number are qualitativly similar. For small values of $1/n_{\mathrm{gs}}$ the energy per particle first decreases and reaches a minimum. For small densities or large volumes, E/N seems to tend to zero. Moreover, we find that the position of the minimum is monotonously shifted to larger densities for increasing N.

The comparison of our DFT-RG results with the exact solution for $N = 2$ suggests that our DFT-RG results are reliable for values of $1/n_{\mathrm{gs}}$ up to about the value where the exact solution assumes a local minimum. For larger values of $1/n_{\mathrm{gs}}$, on the other hand, our present truncation is not capable of recovering the correct scaling behavior of the ground-state energy. However, we can still give an etimate for the ground-state energy in the continuum limit within our present truncation. To do this, we use the fact that the results for the ground-state energy for the two-body problem from our leading-order and next-to-leading-order DFT-RG studies approach the exact result

from above for a given box size L. Moreover, we have found that the exact result approaches the continuum limit from above. We assume now that these two observations also hold for the systems with fermion numbers $N > 2$, we estimate the ground-state energy in the continuum limit from a minimization of E/N with respect to L:

$$E_\infty = \inf_L E(L)\,. \tag{6.34}$$

In Fig. 6.6 we show our leading-order and next-to-leading-order estimates for E_∞/N as a function of N and compare them with the exact result for $N = 2$ and results from Monte Carlo (MC) studies [31] for $N = 4$ and $N = 8$. The error bars of the MC results are smaller than the size of the symbols in Fig. 6.6. In Ref. [31], the ground-state energies in the continuum limit have also been computed in the *Hartree-Fock* approximation for $N = 4, 8, 12$ and found to agree well with the MC data. The continuum-limit result for the ground-state energy of the two-fermion system, which we use as a benchmark for our DFT-RG studies, is neither given for the MC calculation nor the *Hartree-Fock* calculation. However, the MC result presented for $N = 2$ in the presence of a finite volume appears to be in disagreement with our exact solution in the finite box,[7] even on a qualitative level (i. e., the energy from the MC study is found to be negative for $1/n_{\mathrm{gs}} \approx 4.3\,L_0$ rather than positive). In any case, we find that our present best estimate for the ground-state energy of the two-body system underestimates the exact value by about 30%. Moreover, we observe that our results for the ground-state energy per fermion agree on a qualitative level with the available MC results for the continuum limit but the energies from the DFT-RG studies are found to be consistently greater than those from the MC calculations.

[7] This discrepancy may be traced back to differences in the implementation of the two-body interaction in the finite volume. We have studied two possible definitions, see our discussion of Eq. (5.5), and found that the discrepancy between the MC result and our exact solution is present for both implementations of the two-body interaction.

7 Spin-$1/2$ Fermions in a One-Dimensional Box

In this chapter, we study systems of spin-$1/2$ fermions in a one-dimensional periodic box with extent L. We will refer to the two different fermion species as spin-up and spin-down fermions and indicate this with indices $\sigma \in \{\uparrow, \downarrow\}$. More specifically, we study two different types of two-body interaction potentials. In both cases we assume that there is no interaction between fermions with the same spin. In ultracold *Fermi* gases the important process is s-wave scattering and, therefore, it is reasonable to assume fermions with the same spin do not interact with each other. The first two-body potential is the non-local interaction which is repulsive at short distances and attractive at long range, which has already been introduced in the previous chapter in the context of identical fermions. The second is a contact interaction, as it is found in ultracold fermionic systems. Due to the *Pauli* principle the interaction between fermions of the same spin is suppressed for this interaction as discussed above which reflects the situation in dilute ultracold *Fermi* gases [30].

We compute the ground-state energy within our DFT-RG approach up to second order for the non-local potential and up to third order for the contact interaction in an expansion in the small coupling parameter $\bar{g}_N$ for any combination of particle numbers $N_\uparrow$ and $N_\downarrow$. We shall also show that our results agree identically with those obtained by conventional perturbation theory.

We employ our DFT-RG approach to compute ground-state properties of systems with $N_\uparrow$ spin-up fermions and $N_\downarrow$ spin-down fermions, specify the flow equations and introduce the truncations we use in our explicit studies first. In Sec. 7.4 we then show our DFT-RG results for the non-local potential and in Sec. 7.5 we present the results for the contact interaction.

7.1 One-Dimensional Model

In this chapter, we consider systems of spin-$1/2$ fermions in one dimension. We seperate the interaction potential in a space-like part and a spin part:

$$U_{\sigma_1\sigma_2}(x_1, x_2) = U(x_1, x_2)(1 - \delta_{\sigma_1,\sigma_2}). \tag{7.1}$$

This implies that there is no interaction between fermions with the same spin.

For explicit calculations with our DFT-RG approach we use two different two-body interaction potentials U. The first one is the short-range repulsive and long-range attractive two-body interaction potential introduced in the case of identical fermions in Sec. 6.1:

$$U(x_1, x_2) = U_{\mathrm{MC}}(x_1 - x_2). \tag{7.2}$$

In the case of one spin-up and one spin-down fermion it is not possible to calculate the density-density correlation functions and the energy for inverse densities smaller than $1/n_{\mathrm{gs}} \lesssim 30 L_0$, as we will discuss in Sec. 7.3. Therefore, we will consider other values of the coupling constants in this chapter than in the previous one:

$$\bar{g} \equiv g L_0 = 0.6, 1.0 \text{ and } 1.4. \tag{7.3}$$

The second potential we want to use in our studies is a contact interaction given by

$$U(x_1, x_2) = g\, \delta(x_1 - x_2). \tag{7.4}$$

Since we separated the spin part of the interaction potential from the space part, we can study the consequence of this spin part separately. To this end, we consider a potential of the form $U \sim (1-\delta_{\sigma_1,\sigma_2})$. The flow equation of the energy (3.83) contains a term proportional to $\delta_{\sigma_1,\sigma_2}$ and since $(1-\delta_{\sigma_1,\sigma_2})\,\delta_{\sigma_1,\sigma_2} = 0$, this term vanishes and the flow equation for the energy simplifies:

$$\partial_\lambda E_\lambda = \int_{x_1}\int_{x_2} n_{\mathrm{gs},\lambda,\uparrow}(x_1)\,U(x_1-x_2)\,n_{\mathrm{gs},\lambda,\downarrow}(x_2) + \int_{x_1}\int_{x_2} U(x_1-x_2)\,G^{(2)}_{\lambda,\uparrow\downarrow}(0,x_2,0,x_1)\,. \tag{7.5}$$

It is also possible to introduce the Fourier-series representation of the space-like part of the periodically extended interaction potential U as before:

$$U(x_1-x_2) = g\sum_m \mathfrak{U}_{m,m}\,(\phi^{(P)}_m(x_1))^*\phi^{(P)}_m(x_2)\,. \tag{7.6}$$

7.2 Perturbation Theory

In Sec. 3.4 we showed that it is possible to extract perturbative results within our DFT-RG approach. Here, we expand the observables, such as the ground-state energy, in powers of the (small) dimensionless parameter $\bar{g}_N$ also used in Chap. 6:

$$\bar{g}_N = \frac{gL}{N}\,. \tag{7.7}$$

The total ground-state density is homogeneous for any value of λ and is therefore a good property to render the coupling dimensionless.

The zeroth order of the perturbative expansions of the energy, density and the density correlation functions are given by their initial conditions

$$E^{(0)}_{\mathrm{gs}} \equiv \frac{1}{N}E_{\mathrm{gs},\lambda=0}, \quad n^{(0)}_{\mathrm{gs},\sigma} \equiv n_{\mathrm{gs},\lambda=0,\sigma} \quad G^{(2,0)}_{\sigma_1\sigma_2} \equiv G^{(2)}_{\lambda=0,\sigma_1}\,\delta_{\sigma_1,\sigma_2} \quad \text{and} \quad G^{(4,0)}_{\sigma_1\ldots\sigma_4} \equiv G^{(4)}_{\lambda=0,\sigma_1\ldots\sigma_4}\,, \tag{7.8}$$

see Sec. 5.2 for explicit expressions.

Using Eq. (7.5) we observe that the computation of the first-order perturbative correction for the ground-state energy only requires the spin-up and spin-down densities and the up-down-density-density correlation function in their zeroth-order approximations, i. e., $n^{(0)}_{\mathrm{gs},\uparrow}$, $n^{(0)}_{\mathrm{gs},\downarrow}$ and $G^{(2,0)}_{\uparrow\downarrow}$, respectively. Thus, we find

$$\partial_\lambda E^{(1)}_\lambda = \frac{1}{L}\int_{x_1}\int_{x_2} n^{(0)}_{\mathrm{gs},\uparrow}(x_1)\,\mathfrak{U}(x_1-x_2)\,n^{(0)}_{\mathrm{gs},\downarrow}(x_2)\,. \tag{7.9}$$

Since $G^{(2,0)}_{\lambda,\uparrow\downarrow}(\tau_1,x_1,\tau_2,x_2) = 0$, the second term on the right-hand side vanishes and the first-order correction to the energy reads

$$E^{(1)}_{\lambda=1} = \frac{N_\uparrow N_\downarrow}{L^2}\,\mathfrak{U}_{0,0}\,. \tag{7.10}$$

Here, we have used Eq. (5.13). In analogy to the truncation scheme used in Chap. 6, we shall refer to the leading order result of the perturbative expansion as our leading-order DFT-RG result:

$$E^{(LO)}_{\lambda=1} = E_{\mathrm{gs},\lambda=0} + g\,\frac{N_\uparrow N_\downarrow}{L}\,\mathfrak{U}_{0,0}\,. \tag{7.11}$$

To obtain higher-order corrections to the ground-state energy $E_{\mathrm{gs}}^{(n)}$ we plug the expansions (3.80), (3.81) and (3.82) into flow equation (7.5). Since the ground-state density in the interacting case is equal to the initial condition, see Eq. (5.23), all expansion coefficients $n_{\mathrm{gs},\lambda,\sigma}^{(j)} = 0$ for $j \geq 1$. Therefore, the density terms in the flow equations for $E_{\mathrm{gs}}^{(n)}$ vanish. For the term proportional to $G_{\lambda,\uparrow\downarrow}^{(2)}$ in Eq. (7.5), we observe that the $(n-1)$-th order correction of the up-down-density-density correlation function is needed to calculate $E_{\mathrm{gs}}^{(n)}$. We therefore find

$$\partial_\lambda E_\lambda^{(n)} = \frac{n}{L} \int_{x_1} \int_{x_2} \mathfrak{U}(x_1 - x_2)\, G_{\lambda,\uparrow\downarrow}^{(2,n-1)}(0, x_2, 0, x_1) \tag{7.12}$$

for $n \geq 2$.

Now we turn to the computation of the next-to-leading-order correction of the ground-state energy $E_{\mathrm{gs}}^{(2)}$. According to Eq. (7.12) we need the first-order correction of the up-down-density-density correlation function. Therefore, we replace the full correlation functions in Eq. (5.25) by their initial conditions, i. e., $G_{\lambda,\sigma_1,\sigma_2}^{(2)}$ by $G_{\sigma_1\sigma_2}^{(2,0)}$ and $G_{\lambda,\sigma_1\ldots\sigma_4}^{(4)}$ by $G_{\sigma_1\ldots\sigma_4}^{(4,0)}$. The flow equation for $G_{\lambda,\uparrow,\downarrow}^{(2,1)}$ then reads

$$\begin{aligned}\partial_\lambda G_{\lambda,\uparrow\downarrow}^{(2,1)}(\tau_1, x_1, \tau_2, x_2) = &-\frac{N}{L} \int_{\tau_3} \int_{x_3} \int_{x_4} \Big(G_{\uparrow\uparrow}^{(2,0)}(\tau_1, x_1, \tau_3, x_3)\, \mathfrak{U}(x_3 - x_4)\, G_{\downarrow\downarrow}^{(2,0)}(\tau_3, x_4, \tau_2, x_2) \\ &\qquad + G_{\uparrow\downarrow}^{(2,0)}(\tau_1, x_1, \tau_3, x_3)\, \mathfrak{U}(x_3 - x_4)\, G_{\uparrow\downarrow}^{(2,0)}(\tau_3, x_4, \tau_2, x_2) \Big) \\ &- \frac{N}{L} \int_{\tau_3} \int_{x_3} \int_{x_4} \mathfrak{U}(x_3 - x_4)\, G_{\uparrow\downarrow\uparrow\downarrow}^{(4,0)}(\tau_3, x_4, \tau_3, x_3, \tau_1, x_1, \tau_2, x_2)\,. \end{aligned} \tag{7.13}$$

Since the initial conditions for the density correlation functions are equal to zero if not all spin indices are equal, the second and third term on the right-hand side vanish and the flow equation for $G_{\lambda,\uparrow\downarrow}^{(2,1)}$ simplifies considerably:

$$\partial_\lambda G_{\lambda,\uparrow\downarrow}^{(2,1)}(\tau_1, x_1, \tau_2, x_2) = -\frac{N}{L} \int_{\tau_3} \int_{x_3} \int_{x_4} G_{\uparrow\uparrow}^{(2,0)}(\tau_1, x_1, \tau_3, x_3)\, \mathfrak{U}(x_3 - x_4)\, G_{\downarrow\downarrow}^{(2,0)}(\tau_3, x_4, \tau_2, x_2)\,. \tag{7.14}$$

For the leading-order correction $G_{\lambda,\uparrow\downarrow}^{(2,1)}$ we find

$$\begin{aligned} G_{\lambda,\uparrow\downarrow}^{(2,1)}(0, x_1, 0, x_2) = -2\lambda \frac{N}{L^3} \sum_{m\neq 0} \mathfrak{U}_{m,m} \sum_{k,l} &\left(\varepsilon_l^{(I_\downarrow)} - \varepsilon_{l+m}^{(I_\downarrow)} - \varepsilon_k^{(I_\uparrow)} + \varepsilon_{k+m}^{(I_\uparrow)} \right)^{-1} \left(\phi_m^{(\mathrm{p})}(x_1)\right)^* \phi_m^{(\mathrm{p})}(x_2) \\ &\Theta(\bar{\varepsilon}_{\uparrow,k+m}^{(I_\uparrow)}) \Theta(-\bar{\varepsilon}_{\uparrow,k}^{(I_\uparrow)}) \Theta(-\bar{\varepsilon}_{\downarrow,l+m}^{(I_\downarrow)}) \Theta(\bar{\varepsilon}_{\downarrow,l}^{(I_\downarrow)})\,. \end{aligned} \tag{7.15}$$

Here, we give the result for $\tau_1 = \tau_2 = 0$ which is needed to calculate the energy correction.[1]

Using Eq. (7.12) we eventually obtain

$$E_{\lambda=1}^{(2)} = -2\frac{N}{L^4} \sum_{m\neq 0} \mathfrak{U}_{m,m}^2 \sum_{k,l} \left(\varepsilon_l^{(I_\downarrow)} - \varepsilon_{l+m}^{(I_\downarrow)} - \varepsilon_k^{(I_\uparrow)} + \varepsilon_{k+m}^{(I_\uparrow)} \right)^{-1} \Theta(\bar{\varepsilon}_{\uparrow,k+m}^{(I_\uparrow)}) \Theta(-\bar{\varepsilon}_{\uparrow,k}^{(I_\uparrow)}) \Theta(-\bar{\varepsilon}_{\downarrow,l+m}^{(I_\downarrow)}) \Theta(\bar{\varepsilon}_{\downarrow,l}^{(I_\downarrow)})\,. \tag{7.16}$$

We emphasize that this result holds for any combination of particle numbers $N_\uparrow$ and $N_\downarrow$.

[1] See App. C.1 for a detailed calculation.

To obtain the third-order correction to the ground-state energy $E_{gs}^{(3)}$ we need the second-order correction to the up-down-density-density correlation function, see Eq. (7.12). For the flow equation of $G_{\lambda,\uparrow\downarrow}^{(2,2)}$ we find

$$\begin{aligned}\partial_\lambda G_{\lambda,\uparrow\downarrow}^{(2,2)}(\tau_1,x_1,\tau_2,x_2) = -2\frac{N}{L}\int_{\tau_3}\int_{x_3}\int_{x_4}\Big(&G_{\lambda,\uparrow\uparrow}^{(2,1)}(\tau_1,x_1,\tau_3,x_3)\,\mathfrak{U}(x_3-x_4)\,G_{\lambda,\downarrow\downarrow}^{(2,0)}(\tau_3,x_4,\tau_2,x_2)\\ &+G_{\lambda,\uparrow\downarrow}^{(2,1)}(\tau_1,x_1,\tau_3,x_3)\,\mathfrak{U}(x_3-x_4)\,G_{\lambda,\uparrow\downarrow}^{(2,0)}(\tau_3,x_4,\tau_2,x_2)\\ &+G_{\lambda,\uparrow\uparrow}^{(2,0)}(\tau_1,x_1,\tau_3,x_3)\,\mathfrak{U}(x_3-x_4)\,G_{\lambda,\downarrow\downarrow}^{(2,1)}(\tau_3,x_4,\tau_2,x_2)\\ &+G_{\lambda,\uparrow\downarrow}^{(2,0)}(\tau_1,x_1,\tau_3,x_3)\,\mathfrak{U}(x_3-x_4)\,G_{\lambda,\uparrow\downarrow}^{(2,1)}(\tau_3,x_4,\tau_2,x_2)\Big)\\ &-2\frac{N}{L}\int_{\tau_3}\int_{x_3}\int_{x_4}\mathfrak{U}(x_3-x_4)\,G_{\uparrow\downarrow\uparrow\downarrow}^{(4,1)}(\tau_3,x_4,\tau_3,x_3,\tau_1,x_1,\tau_2,x_2)\,. \end{aligned} \tag{7.17}$$

The second and the fourth term vanish because $G_{\lambda,\uparrow\downarrow}^{(2,0)}=0$. For the first and third term we look at the first-order corrections of the up-up- and the down-down-density-density correlation functions. The flow equations for $G_{\lambda,\uparrow\uparrow}^{(2,1)}$ and $G_{\lambda,\downarrow\downarrow}^{(2,1)}$ read

$$\begin{aligned}\partial_\lambda G_{\lambda,\sigma\sigma}^{(2,1)}(\tau_1,x_1,\tau_2,x_2) = -2\frac{N}{L}\int_{\tau_3}\int_{x_3}\int_{x_4}&G_{\sigma\sigma}^{(2,0)}(\tau_1,x_1,\tau_3,x_3)\,\mathfrak{U}(x_3-x_4)\,G_{\uparrow\downarrow}^{(2,0)}(\tau_3,x_4,\tau_2,x_2)\\ &-\frac{N}{L}\int_{\tau_3}\int_{x_3}\int_{x_4}\mathfrak{U}(x_3-x_4)\,G_{\lambda,\uparrow\downarrow\sigma\sigma}^{(4,1)}(\tau_3,x_4,\tau_3,x_3,\tau_1,x_1,\tau_2,x_2)\,. \end{aligned} \tag{7.18}$$

These flow equations both vanish since the initial conditions of $G_{\uparrow\downarrow}^{(2,0)}$ and $G_{\uparrow\downarrow\sigma\sigma}^{(4,0)}$ are equal to zero and we find

$$G_{\lambda,\uparrow\uparrow}^{(2,1)}(\tau_1,x_1,\tau_2,x_2)=0 \quad\text{and}\quad G_{\lambda,\downarrow\downarrow}^{(2,1)}(\tau_1,x_1,\tau_2,x_2)=0\,. \tag{7.19}$$

Therefore, also the first and the third term in Eq. (7.17) vanish at order g^2 and the flow equation for the second-order correction of the up-down-density-density correlation function simplifies considerably:

$$\partial_\lambda G_{\lambda,\uparrow\downarrow}^{(2,2)}(\tau_1,x_1,\tau_2,x_2) = -2\frac{N}{L}\int_{\tau_3}\int_{x_3}\int_{x_4}\mathfrak{U}(x_3-x_4)\,G_{\lambda,\uparrow\downarrow\uparrow\downarrow}^{(4,1)}(\tau_3,x_4,\tau_3,x_3,\tau_1,x_1,\tau_2,x_2)\,. \tag{7.20}$$

To obtain the leading-order correction of $G_{\lambda,\uparrow\downarrow\uparrow\downarrow}^{(4,1)}$ we have to plug the initial conditions of the density correlation functions into the flow equation (3.77). Since only the initial conditions of the density correlation functions with equal spin indices are non-zero, only one term remains in the flow equation and we find

$$\begin{aligned}&\partial_\lambda G_{\lambda,\uparrow\downarrow\uparrow\downarrow}^{(4,1)}(\tau_1,x_1,\tau_2,x_2,\tau_3,x_3,\tau_4,x_4)\\ &\qquad=-\frac{N}{L}\int_{\tau_5}\int_{x_5}\int_{x_6}G_{\uparrow\uparrow\uparrow}^{(3,0)}(\tau_1,x_1,\tau_3,x_3,\tau_5,x_5)\,\mathfrak{U}(x_5-x_6)\,G_{\downarrow\downarrow\downarrow}^{(3,0)}(\tau_5,x_6,\tau_2,x_2,\tau_4,x_4)\,. \end{aligned} \tag{7.21}$$

To obtain now the third-order correction of the ground-state energy, we recall that it suffices to calculate the density-density correlation function $G_{\lambda,\uparrow\downarrow}^{(2,2)}$ for $\tau_1=\tau_2=0$. We find

$$\begin{aligned}&G_{\lambda,\uparrow\downarrow}^{(2,2)}(0,x_1,0,x_2)\\ &\quad=\lambda^2\left(\frac{N}{L}\right)^2\int_{\tau_3}\int_{x_3}\int_{x_4}\mathfrak{U}(x_3-x_4)\int_{\tau_5}\int_{x_5}\int_{x_6}G_{\uparrow\uparrow\uparrow}^{(3,0)}(\tau_3,x_3,0,x_1,\tau_5,x_5)\,\mathfrak{U}(x_5-x_6)\,G_{\downarrow\downarrow\downarrow}^{(3,0)}(\tau_5,x_6,\tau_3,x_4,0,x_2)\,. \end{aligned} \tag{7.22}$$

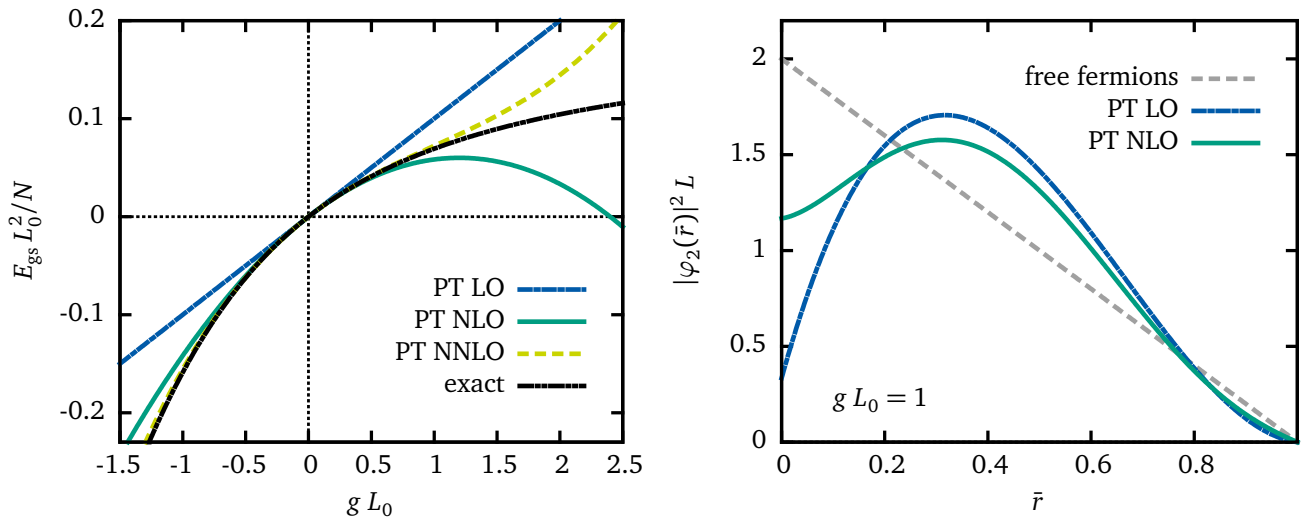

Figure 7.1.: Results of the perturbative expansion obtained within our DFT-RG framework. Left panel: Ground-state energy per fermion as a function of the coupling strength up to the third-order perturbative result in comparison with the exact solution. Right panel: Dimensionless absolute square of the ground-state wavefunction $|\varphi_2(\bar{r})|^2\,L$ in the center-of-mass frame as a function of $\bar{r} = r/L$ up to second order in the perturbative expansion in comparison with the result of the non-interacting system.

This expression can be used to obtain the second-order correction to the up-down-density-density correlation functions for any potential. For convenience we give here only the result for the contact interaction for one spin-up and one spin-down fermion:[2]

$$\begin{aligned} G^{(2,2)}_{\lambda,\uparrow\downarrow}(0,x_1,0,x_2) = {} & \frac{\lambda^2}{L^3}\left(\frac{N}{L}\right)^2 \sum_{k_1\neq 0}\sum_{k_3\neq 0} \frac{1}{\varepsilon^{(\mathrm{P})}_{k_1}} \frac{1}{\varepsilon^{(\mathrm{P})}_{k_3}} (\phi^{(\mathrm{P})}_{k_3}(x_1))^* \phi^{(\mathrm{P})}_{k_3}(x_2) \\ & - \frac{\lambda^2}{L^3}\left(\frac{N}{L}\right)^2 \sum_{k_2\neq 0} \frac{1}{(\varepsilon^{(\mathrm{P})}_{k_2})^2} (\phi^{(\mathrm{P})}_{k_2}(x_2))^* \phi^{(\mathrm{P})}_{k_2}(x_1) \\ & + \frac{\lambda^2}{2L^2}\left(\frac{N}{L}\right)^2 \sum_{k_2\neq 0}\sum_{k_3\neq 0} \frac{1}{\varepsilon^{(\mathrm{P})}_{k_2}} \frac{1}{\varepsilon^{(\mathrm{P})}_{k_3}} (\phi^{(\mathrm{P})}_{k_2}(x_2))^* \phi^{(\mathrm{P})}_{k_2}(x_1) (\phi^{(\mathrm{P})}_{k_3}(x_1))^* \phi^{(\mathrm{P})}_{k_3}(x_2) \\ & - \frac{\lambda^2}{2L^4}\left(\frac{N}{L}\right)^2 \sum_{k_1\neq 0} \frac{1}{(\varepsilon^{(\mathrm{P})}_{k_1})^2}\,. \end{aligned} \tag{7.23}$$

Using the result for $G^{(2,2)}_{\lambda,\uparrow\downarrow}$ and Eq. (7.12), we can then obtain the third-order correction for the ground-state energy $E^{(3)}_{\mathrm{gs}}$. For a contact interaction of the form (7.4) we find for one spin-up and one spin-down fermion

$$E^{(3)}_{\mathrm{gs}} = \frac{4}{L^2}\frac{6}{180}\,. \tag{7.24}$$

Overall, we find for the two-body system

$$E_{\mathrm{gs}} = 2\left(\frac{1}{L^2}\,\bar{g}_N - \frac{2}{L^2}\frac{1}{12}\,\bar{g}_N^2 + \frac{4}{L^2}\frac{1}{180}\,\bar{g}_N^3 + \mathcal{O}(\bar{g}_N^4)\right), \tag{7.25}$$

which agrees identically with the result obtained by conventional perturbation theory.

As an illustration of this result we show the ground-state energy per fermion as a function of the coupling strength for different orders of the perturbative expansion in the left panel of Fig. 7.1.

[2] See App. C.2 for the expression for $G^{(2,2)}_{\lambda,\uparrow\downarrow}(0,x_1,0,x_2)$ for any combination of particle numbers in case of a contact interaction.

In the case of one spin-up and one spin-down fermion we can also calculate the perturbative corrections for the two-body wavefunction. Using Eqs. (3.52), (3.84) and (7.15) we find for the leading-order correction

$$|\Psi_{\mathrm{gs}}^{(1)}(x_1,x_2)|^2 = G^{(2,1)}_{\lambda=1,\uparrow\downarrow}(0,x_1,0,x_2) = -\frac{2}{L^3}\sum_{m\neq 0}\mathfrak{U}_{m,m}\frac{1}{\varepsilon_m^{(\mathrm{P})}}\,(\phi_m^{(\mathrm{P})}(x_1))^*\,\phi_m^{(\mathrm{P})}(x_2) \tag{7.26}$$

and using Eq. (7.23) we can obtain the next-to-leading order correction

$$|\Psi_{\mathrm{gs}}^{(2)}(x_1,x_2)|^2 = G^{(2,2)}_{\lambda=1,\uparrow\downarrow}(0,x_1,0,x_2)\,. \tag{7.27}$$

With these results the perturbative expansion of the absolute square of the wavefunction can be reconstructed, see Eq. (3.84). Using Eq. (3.53), the results for the intrinsic density of the small-coupling expansion can be obtained. To illustrate this we show the result for the leading-order and next-to-leading-order perturbative approximation for the intrinsic density in the right panel of Fig. 7.1.

Note that the reconstruction of the perturbative series from our DFT-RG approach can be systematically continued to higher orders in the dimensionless coupling g_N , as already mentioned in the chapter about systems of identical fermions.

7.3 DFT-RG Flow Equations

In this section, we discuss the flow equations and their truncations which we use for our explicit studies. To define these truncations we again use the results of our previous discussions about our DFT-RG approach and the connection to many-body perturbation theory. Using Eqs. (7.5) and (7.10), we find the following differential equation for the ground-state energy:

$$\frac{1}{N}\partial_\lambda E_\lambda = \bar{g}_N\,\frac{N_\uparrow N_\downarrow}{L^2}\,\mathfrak{U}_{0,0} + \frac{\bar{g}_N}{L}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\sum_a \mathfrak{U}_{a,a}\,\tilde{G}^{(2)}_{\lambda,\uparrow\downarrow,a,a}(\omega)\,, \tag{7.28}$$

where we have introduced the Fourier transform of the density-density correlation function $G^{(2)}_{\lambda,\sigma_1\sigma_2}$,

$$G^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1,x_1,\tau_2,x_2) = \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\sum_{a,b}\tilde{G}^{(2)}_{\lambda,\sigma_1\sigma_2,a,b}(\omega)\,(\phi_a^{(\mathrm{P})}(x_1))^*\,\phi_b^{(\mathrm{P})}(x_2)\,\mathrm{e}^{-\mathrm{i}\omega(\tau_1-\tau_2)}\,. \tag{7.29}$$

The initial condition of this flow equation is given by the energy of the non-interacting system of $N_\uparrow$ spin-up fermions and $N_\downarrow$ spin-down fermions, see Eq. (5.7).

As discussed above, the flow equations for the spin densities are equal to zero. Thus, we get directly to the flow equations for the density-density correlation functions. The exact flow equations for the density-density correlation functions $G^{(2)}_{\lambda,\sigma_1\sigma_2}$ read

$$\begin{aligned}\partial_\lambda G^{(2)}_{\lambda,\sigma_1\sigma_2}(\tau_1,x_1,\tau_2,x_2) = &-\int_{\tau_3}\int_{x_3}\int_{x_4} G^{(2)}_{\lambda,\sigma_1\uparrow}(\tau_1,x_1,\tau_3,x_3)\,U(x_3-x_4)\,G^{(2)}_{\lambda,\downarrow\sigma_2}(\tau_3,x_4,\tau_2,x_2)\\ &-\int_{\tau_3}\int_{x_3}\int_{x_4} G^{(2)}_{\lambda,\sigma_1\downarrow}(\tau_1,x_1,\tau_3,x_3)\,U(x_3-x_4)\,G^{(2)}_{\lambda,\uparrow\sigma_2}(\tau_3,x_4,\tau_2,x_2)\\ &-\int_{\tau_3}\int_{x_3}\int_{x_4} U(x_3-x_4)\,G^{(4)}_{\lambda,\uparrow\downarrow\sigma_1\sigma_2}(\tau_3,x_4,\tau_3,x_3,\tau_1,x_1,\tau_2,x_2)\,.\end{aligned} \tag{7.30}$$

In analogy to the discussion in the previous chapter about identical fermions, we shall neglect the flow for all correlation functions $G^{(n)}_{\lambda,\sigma_1\ldots\sigma_n}$ with $n>2$. We note that in the last term the first two spin indices of $G^{(4)}_{\lambda,\uparrow\downarrow\sigma_1\sigma_2}$ are always different. If we replace the full four-density correlation function appearing in this flow equation by the

initial condition $G^{(4)}_{\lambda=0,\uparrow\downarrow\sigma_1\sigma_2} = 0$, this term vanishes. In Sec. 7.2, we have discussed that we obtain the exact second-order perturbative correction if we also replace the density-density correlation functions by their initial conditions in Eq. (7.30). By solving the differential equations (7.30) with the full density-density correlation functions we indeed take into account arbitrarily high orders in the dimensionless coupling parameter $\bar{g}_N$. Thus, we are left with the first two terms of Eq. (7.30) to define the next-to-leading-order truncation within our DFT-RG framework.

Using the Fourier transform defined by Eq. (7.29), we find the following set of flow equations for the density-density correlation functions:

$$\partial_\lambda \tilde{G}^{(2)}_{\lambda,\uparrow\uparrow,a,a}(\omega) = -2\,g\,\tilde{G}^{(2)}_{\lambda,\uparrow\uparrow,a,a}(\omega)\,\mathfrak{U}_{a,a}\,\tilde{G}^{(2)}_{\lambda,\uparrow\downarrow,a,a}(\omega) \tag{7.31}$$

$$\partial_\lambda \tilde{G}^{(2)}_{\lambda,\downarrow\downarrow,a,a}(\omega) = -2\,g\,\tilde{G}^{(2)}_{\lambda,\downarrow\downarrow,a,a}(\omega)\,\mathfrak{U}_{a,a}\,\tilde{G}^{(2)}_{\lambda,\uparrow\downarrow,a,a}(\omega) \tag{7.32}$$

$$\partial_\lambda \tilde{G}^{(2)}_{\lambda,\uparrow\downarrow,a,a}(\omega) = -g\,\left(\tilde{G}^{(2)}_{\lambda,\uparrow\uparrow,a,a}(\omega)\,\mathfrak{U}_{a,a}\,\tilde{G}^{(2)}_{\lambda,\downarrow\downarrow,a,a}(\omega) + \tilde{G}^{(2)}_{\lambda,\uparrow\downarrow,a,a}(\omega)\,\mathfrak{U}_{a,a}\,\tilde{G}^{(2)}_{\lambda,\uparrow\downarrow,a,a}(\omega)\right) \tag{7.33}$$

This set of flow equations can be solved analytically and we find

$$\tilde{G}^{(2)}_{\lambda,\uparrow\uparrow,a,a}(\omega) = -\frac{\tilde{G}^{(2)}_{0,\uparrow\uparrow,a,a}(\omega)}{\lambda^2\,g^2\,\mathfrak{U}^2_{a,a}\,\tilde{G}^{(2)}_{0,\uparrow\uparrow,a,a}(\omega)\,\tilde{G}^{(2)}_{0,\downarrow\downarrow,a,a}(\omega) - 1}\,, \tag{7.34}$$

$$\tilde{G}^{(2)}_{\lambda,\downarrow\downarrow,a,a}(\omega) = -\frac{\tilde{G}^{(2)}_{0,\downarrow\downarrow,a,a}(\omega)}{\lambda^2\,g^2\,\mathfrak{U}^2_{a,a}\,\tilde{G}^{(2)}_{0,\uparrow\uparrow,a,a}(\omega)\,\tilde{G}^{(2)}_{0,\downarrow\downarrow,a,a}(\omega) - 1}\,, \tag{7.35}$$

$$\tilde{G}^{(2)}_{\lambda,\uparrow\downarrow,a,a}(\omega) = \frac{\lambda\,g\,\mathfrak{U}_{a,a}\,\tilde{G}^{(2)}_{0,\uparrow\uparrow,a,a}(\omega)\tilde{G}^{(2)}_{0,\downarrow\downarrow,a,a}(\omega)}{\lambda^2\,g^2\,\mathfrak{U}^2_{a,a}\,\tilde{G}^{(2)}_{0,\uparrow\uparrow,a,a}(\omega)\,\tilde{G}^{(2)}_{0,\downarrow\downarrow,a,a}(\omega) - 1}\,, \tag{7.36}$$

where

$$\tilde{G}^{(2)}_{0,\sigma\sigma,a,a}(\omega) = \frac{2}{L}\sum_k \theta(\bar{\varepsilon}^{(I_\sigma)}_{\sigma,k})\theta(-\bar{\varepsilon}^{(I_\sigma)}_{\sigma,k-a})\frac{|\varepsilon^{(I_\sigma)}_{\sigma,k} - \varepsilon^{(I_\sigma)}_{\sigma,k-a}|}{\omega^2 + |\varepsilon^{(I_\sigma)}_{\sigma,k} - \varepsilon^{(I_\sigma)}_{\sigma,k-a}|^2} \tag{7.37}$$

is the a-th Fourier coefficient of the density-density correlation functions of the non-interacting system. We shall refer to this solution as the next-to-leading-order DFT-RG approximation. Note that all Fourier coefficients of the density-density correlation functions have a singularity at $\lambda^2\,g^2\,\mathfrak{U}^2_{a,a}\,\tilde{G}^{(2)}_{0,\uparrow\uparrow,a,a}(\omega)\,\tilde{G}^{(2)}_{0,\downarrow\downarrow,a,a}(\omega) = 1$.

If we now plug the result for $G^{(2)}_{\lambda,\uparrow\downarrow,a,a}(\omega)$ given by Eq. (7.36) into the flow equation for the energy (7.28) we obtain the next-to-leading-order DFT-RG result for the ground-state energy

$$E_{\lambda=1} = \frac{\pi^2}{6\,L^2}\left(N_\uparrow^3 + N_\downarrow^3 - N\right) + g\,N_\uparrow N_\downarrow\frac{\mathfrak{U}_{0,0}}{L} + \frac{1}{2}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\sum_{a\neq 0}\ln\left(1 - g^2\,\mathfrak{U}^2_{a,a}\,\tilde{G}^{(2)}_{0,\uparrow\uparrow,a,a}(\omega)\,\tilde{G}^{(2)}_{0,\downarrow\downarrow,a,a}(\omega)\right), \tag{7.38}$$

where the first term is the energy of the non-interacting system given by Eq. (5.7). We note that this result for the energy has a singularity at $g^2\,\mathfrak{U}^2_{a,a}\,\tilde{G}^{(2)}_{0,\uparrow\uparrow,a,a}(\omega)\,\tilde{G}^{(2)}_{0,\downarrow\downarrow,a,a}(\omega) = 1$, which is a consequence of the divergence appearing in $G^{(2)}_{\lambda,\uparrow\downarrow}$. For a given interaction strength g this divergence effectively restricts the box sizes L that can be calculated or vice versa. This behavior is due to the used approximation and not a problem of the DFT approach itself. Taking higher-order flow equations into account fixes the singularity.

In Fig. 7.2, we show the term $\mathfrak{U}^2_{a,a}\,\tilde{G}^{(2)}_{0,\uparrow\uparrow,a,a}(\omega)\,\tilde{G}^{(2)}_{0,\downarrow\downarrow,a,a}(\omega)$ for $a = 1$ and $\omega = 0$, which represents an upper bound for the family of functions with different values of a. It is not possible to obtain a result for a given box size L if the term $\mathfrak{U}^2_{a,a}\,\tilde{G}^{(2)}_{0,\uparrow\uparrow,a,a}(\omega)\,\tilde{G}^{(2)}_{0,\downarrow\downarrow,a,a}(\omega)$ is larger than the inverse square of the interaction strength $1/g^2$. We notice that in the case of the non-local potential it is possible to obtain results for all box sizes for coupling constants $g\,L_0 \lesssim 1.48$. In the case of the contact interaction there is no value for the interaction strength g for which we can study all box sizes in the current approximation.

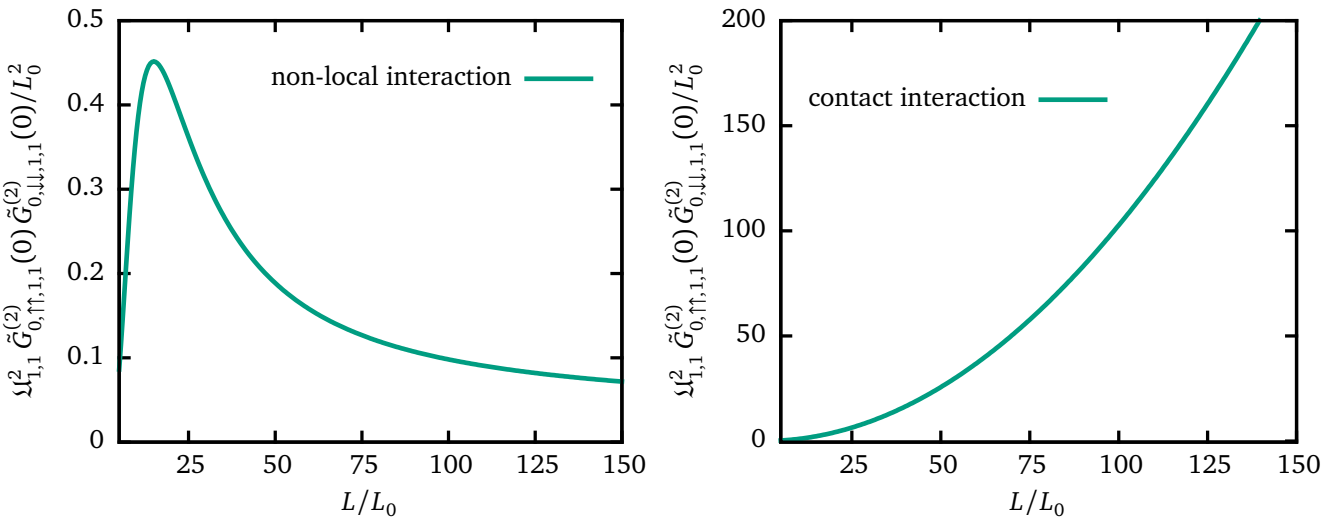

Figure 7.2.: Size of the term $\mathfrak{U}_{a,a}^2\,\tilde{G}^{(2)}_{0,\uparrow\uparrow,a,a}(\omega)\,\tilde{G}^{(2)}_{0,\downarrow\downarrow,a,a}(\omega)$ appearing in the denominator of $\tilde{G}^{(2)}_{\lambda,\downarrow\downarrow,a,a}(\omega)$, see Eqs. (7.34), (7.35) and (7.36), as a function of the box size. We only show this term for $a = 1$ and $\omega = 0$, which represents an upper bound for $a \neq 1$.

We also point to a peculiarity of this truncation. Expanding the function $\ln(1-x)$ about $x = 0$ yields

$$\ln(1-x) = -\sum_{k=1}^{\infty} \frac{x^k}{k}\,. \tag{7.39}$$

The coupling g appears quadratic in the logarithm, see Eq. (7.38), therefore only even powers in g are generated in this approximation. This already explains to some extent the appearence of a divergence as odd powers of g are present in a perturbative expansion, see Eq. (7.25).

Let us now consider an improvement to the next-to-leading-order DFT-RG approximation in the case of the contact interaction. Since the initial condition of the density-density correlation function $G^{(4)}_{\lambda=0,\uparrow\downarrow\sigma_1\sigma_2}$ is equal to zero we would like to include its leading-order perturbative correction in the flow equation. It is very involved to calculate the time-dependent leading-order correction for the four-density correlator. For a first improvement of our flow equations we therefore only include the term with the four-density correlation function $G^{(4,1)}_{\lambda,\uparrow\downarrow\uparrow\downarrow}$ that is needed to obtain the correct third-order perturbative correction for the energy, see our discussion in Sec. 7.2. This means that we do not change the flow equations for $G^{(2)}_{\lambda,\uparrow\uparrow}$ and $G^{(2)}_{\lambda,\downarrow\downarrow}$ but only the flow equation for $G^{(2)}_{\lambda,\uparrow\downarrow}$. We replace the last term on the right-hand side of Eq. (7.30) for $G^{(2)}_{\lambda,\uparrow\downarrow}$ as follows:

$$\begin{aligned} &-\int_{\tau_3}\int_{x_3}\int_{x_4} U(x_3-x_4)\,G^{(4)}_{\lambda,\uparrow\downarrow\uparrow\downarrow}(\tau_3,x_4,\tau_3,x_3,\tau_1,x_1,\tau_2,x_2) \\ &\quad\to\quad -\int_{\tau_3}\int_{x_3}\int_{x_4} U(x_3-x_4)\,G^{(4,1)}_{\lambda,\uparrow\downarrow\uparrow\downarrow}(\tau_3,x_4,\tau_3,x_3,0,x_1,0,x_2) \equiv \mathscr{G}^{(4,2)}_{\lambda,\uparrow\downarrow}(x_1,x_2)\,. \end{aligned} \tag{7.40}$$

To use this term in numerical calculations we have to perform a Fourier transformation. Note that $\mathscr{G}^{(4,2)}_{\lambda,\uparrow\downarrow}(x_1,x_2)$ is time independent since we evaluated this term only at $\tau_1 = \tau_2 = 0$. Therefore, the Fourier transformation is proportional to $\delta(\omega)$ and the flow for the up-down-density-density correlation function reads:

$$\partial_\lambda \tilde{G}^{(2)}_{\lambda,\uparrow\downarrow,a,a}(\omega) = -g\left(\tilde{G}^{(2)}_{\lambda,\uparrow\uparrow,a,a}(\omega)\,\mathfrak{U}_{a,a}\,\tilde{G}^{(2)}_{\lambda,\downarrow\downarrow,a,a}(\omega) + \tilde{G}^{(2)}_{\lambda,\uparrow\downarrow,a,a}(\omega)\,\mathfrak{U}_{a,a}\,\tilde{G}^{(2)}_{\lambda,\uparrow\downarrow,a,a}(\omega) + 2\pi\,\tilde{\mathscr{G}}^{(4,2)}_{\lambda,\uparrow\downarrow,a,a}\,\delta(\omega)\right), \tag{7.41}$$

where

$$\mathscr{G}^{(4,2)}_{\lambda,\uparrow\downarrow}(x_1,x_2) = \sum_{a,b} \tilde{\mathscr{G}}^{(4,2)}_{\lambda,\uparrow\downarrow,a,b}\,(\phi^{(\mathrm{P})}_a(x_1))^*\,\phi^{(\mathrm{P})}_b(x_2)\,. \tag{7.42}$$

For one spin-up and one spin-down particle we find for example

$$\tilde{\mathcal{G}}^{(4,2)}_{\lambda,\uparrow\downarrow,a,a} = \begin{cases} 0 & \text{for } a = 0\,, \\ \lambda\, g^2\, L\, \frac{-7+a^2\pi^2}{4a^4\pi^4} & \text{otherwise}\,. \end{cases} \tag{7.43}$$

To solve the set of flow equations (7.28) and (7.41) we again introduce a cutoff Λ_F for the Fourier modes. We checked the convergence of our results and found that a combination of the cutoff values of $\Lambda_\mathrm{F} = 50$ for the Fourier modes and $\Lambda_\mathrm{C} = 50$ for the *Chebyshev* nodes suffices in the case of one spin-up and one spin-down fermion. To perform the integrations over ω we use the *Chebyshev-Gauss* quadrature detailed in Sec. 6.4. Therefore, we have to define how we want to treat the δ-distribution in the numerical calculations. We introduce a θ-function to approximate the δ-distribution such that the integration over the θ-function yields unity:

$$\int_{-\infty}^{\infty} \mathrm{d}\omega\; \delta(\omega) = 1 \quad \rightarrow \quad \int_{-\infty}^{\infty} \mathrm{d}\omega\; \Theta(c^2 - \omega^2)\, \frac{1}{2c} = 1\,, \tag{7.44}$$

where we determine the constant c such that the width of the θ-function includes only the two *Chebyshev* nodes $\tilde{\omega}_i$ right and left of $\omega = 0$:

$$\tilde{\omega}_{\Lambda_\mathrm{C}/2} = \cos\left(\frac{\Lambda_\mathrm{C}-1}{2\,\Lambda_\mathrm{C}}\pi\right) \quad \text{and} \quad \tilde{\omega}_{\Lambda_\mathrm{C}/2+1} = \cos\left(\frac{\Lambda_\mathrm{C}+1}{2\,\Lambda_\mathrm{C}}\pi\right). \tag{7.45}$$

We assume here that we always use an even number of *Chebyshev* nodes Λ_C. We find

$$c = \tan\left(\frac{\pi}{2}\cos\left(\frac{\Lambda_\mathrm{C}-1}{2\,\Lambda_\mathrm{C}}\pi\right)\right). \tag{7.46}$$

The flow equation for the up-down-density-density correlation function used in our numerical studies then reads

$$\begin{aligned} \partial_\lambda \tilde{G}^{(2)}_{\lambda,\uparrow\downarrow,a,a}(\tilde{\omega}_i) = &- g\,\left(\tilde{G}^{(2)}_{\lambda,\uparrow\uparrow,a,a}(\tilde{\omega}_i)\,\mathfrak{U}_{a,a}\,\tilde{G}^{(2)}_{\lambda,\downarrow\downarrow,a,a}(\tilde{\omega}_i) + \tilde{G}^{(2)}_{\lambda,\uparrow\downarrow,a,a}(\tilde{\omega}_i)\,\mathfrak{U}_{a,a}\,\tilde{G}^{(2)}_{\lambda,\uparrow\downarrow,a,a}(\tilde{\omega}_i)\right) \\ &- g\,\frac{2\,\pi}{2\,c}\,\tilde{\mathcal{G}}^{(4,2)}_{\lambda,\uparrow\downarrow,a,a}\left(\delta_{i,\Lambda_C/2} + \delta_{i,\Lambda_C/2+1}\right). \end{aligned} \tag{7.47}$$

We will refer to this as the improved next-to-leading-order DFT-RG equation. Using flow equation (7.47) instead of flow equation (7.30) indeed improves the results for the energy, as we will see in Sec. 7.5. This approximation is, nevertheless, not able to push the singularity to higher values of the interaction strength g.

To show that this is not a problem of our DFT-RG framework but of the used truncation, we would like to motivate that it is possible to improve our results if we take a better approximation of $\tilde{\mathcal{G}}^{(4,2)}_{\lambda,\uparrow\downarrow}$ into account. We note that $\tilde{\mathcal{G}}^{(4,2)}_{\lambda,\uparrow\downarrow,a,a} \sim \lambda$. To improve our results we can replace

$$\tilde{\mathcal{G}}^{(4,2)}_{\lambda,\uparrow\downarrow,a,a} \quad \rightarrow \quad (1 + f(g,L)\,\lambda)\,\tilde{\mathcal{G}}^{(4,2)}_{\lambda,\uparrow\downarrow,a,a} \tag{7.48}$$

in Eq. (7.47) to include a factor of λ^2. This corresponds to an expansion of the term proportional to $G^{(4)}_{\lambda,\uparrow\downarrow\uparrow\downarrow}$ in powers of λ. The function $f(g,L)$ can be adjusted in the case of one spin-up and one spin-down fermion to reproduce the result of the exactly solvable two-body problem, see Sec. 7.5. In a next step, this function could then be used in the flow equations for higher particle numbers to improve these results.

In this thesis, we shall perform a feasibility study of this approach for the case of two fermions. We will show that it is possible to find a function $f(g,L)$ to reproduce the exact two-body result. In the case of higher fermion numbers we restrict the studies in this thesis to the next-to-leading-order result and defer a study of the improved next-to-leading-order approximation to future work.

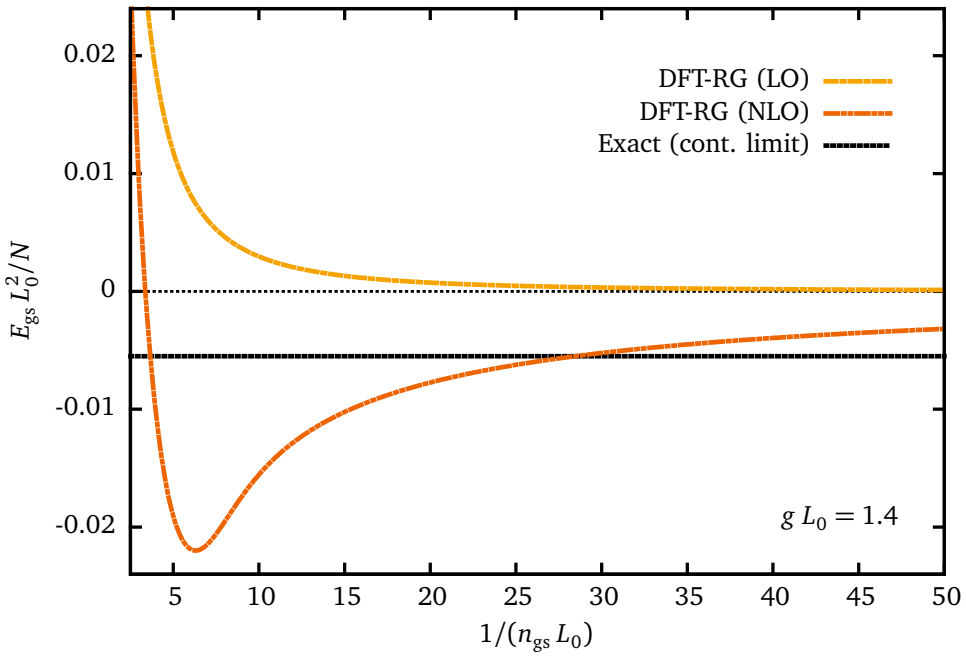

Figure 7.3.: Ground-state energy per fermion of the two-body problem with one spin-up and one spin-down fermion as a function of the inverse ground-state density for a coupling constant $g\,L_0 = 1.4$ as obtained by different approaches.

7.4 DFT-RG Results – Non-Local Potential

Let us now discuss the results for a non-local potential. In this section we show the results for the short-range repulsive and long-range attractive two-body interaction

$$U_{\mathrm{MC}}(x_1 - x_2) = \frac{g}{\sigma_1\sqrt{\pi}}\,\mathrm{e}^{-\frac{(x_1-x_2)^2}{\sigma_1^2}} - \frac{g}{\sigma_2\sqrt{\pi}}\,\mathrm{e}^{-\frac{(x_1-x_2)^2}{\sigma_2^2}}\,, \tag{7.49}$$

see Sec. 6.1 for an introduction of the potential and the parameters. For the coupling constant we choose different values here, see our discussion above:

$$\bar{g} \equiv g\,L_0 = 0.6\,, 1.0 \text{ and } 1.4\,. \tag{7.50}$$

In Figs. 7.3 and 7.4, we show the ground-state energy per fermion E/N of the two-body problem with one spin-up and one spin-down fermion as a function of the inverse ground-state density. We would like to mention again that the density $n_{gs} = N/L$ should by no means be confused with the intrinsic density of the system that can be extracted for two fermions from the density-density correlation function, see Eqs. (3.52) and (3.53).

In Fig. 7.3, the results as obtained from our DFT-RG framework for $g\,L_0 = 1.4$ are shown, namely the result from our DFT-RG approach in the leading-order approximation (LO) as given by Eq. (7.11) and in the next-to-leading-order approximation (NLO) as discussed in Sec. 7.3. For comparison we also show the exact result of the ground-state energy in the continuum limit obtained by solving the *Schrödinger* equation in the center-of-mass frame in a sufficiently large subspace spanned by harmonic oscillator eigenfunctions.

We observe that the leading-order DFT-RG approximation is always larger than zero, which is already clear from the fact that $\mathfrak{U}_{0,0} > 0$ for all values of L and $\mathfrak{U}_{0,0} \to 0$ in the limit $L \to \infty$. Since the energy of the non-interaction system is equal to zero, the leading-order approximation is proportional to $\mathfrak{U}_{0,0}/L$ which explains the rapid decrease of

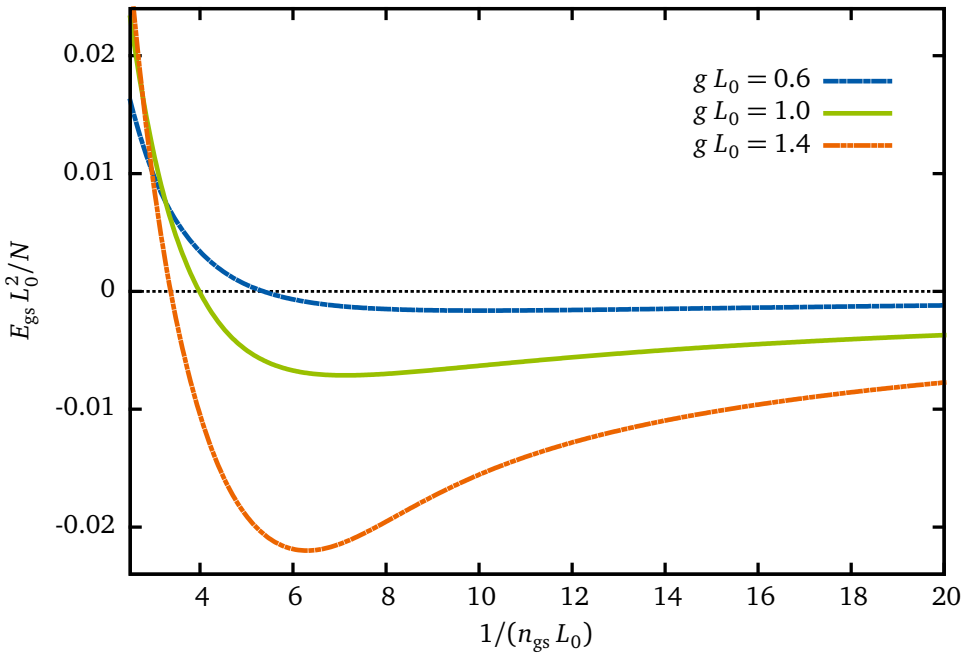

Figure 7.4.: Ground-state energy per fermion of the two-body problem with one spin-up and one spin-down fermion as a function of the inverse ground-state density in DFT-RG NLO for different coupling constants g.

this result as a function of L. The results obtained from our DFT-RG approach in leading order deviate significantly from the results obtained at next-to-leading order on the complete range of the plot, even for small box sizes. On a qualitative level the two-body energy in the next-to-leading-order DFT-RG approximation assumes a similar structure as in the case of two identical fermions, as one would expect. In the system of two fermions with different spins, the energy has a minimum for small box sizes or large densities that assumes smaller values for E/N compared to the case of identical fermions, even though the coupling constant used in this case is smaller. In the limit $L \to \infty$ the next-to-leading-order approximation converges to zero from below and cannot reproduce the continuum-limit result $E/N|_{\rm cont.} \approx -0.0055\,(1/L_0^2)$. The perturbative expansion has alternating signs for each power of g. Since we construct our truncations in accordance to the perturbative expansion we may assume that the next-to-next-to-leading-order DFT-RG approximation assumes for small box sizes or large densities values in between the leading-order and the next-to-leading-order results. If this assumption holds it could be possible to use the minimum of the DFT-RG results to obtain a lower bound for the continuum energy. For a rigorous proof of this conjecture, higher-order calculations would be necessary.

In Fig. 7.4, we show results for the ground-state energy per particle for three different values of the coupling constant as obtained by our next-to-leading-order DFT-RG approximation. The qualitative behavior for all values of g is similar, each curve assumes a minimum for small box sizes or large densities and tends to zero in the limit $L \to \infty$ and, therefore, fails to reproduce the energy in the continuum limit.[3] The values of the inverse density for which the energy becomes negative is shifted to larger densities for larger couplings. For $g\,L_0 = 0.6$ the zero crossing is at $1/n_{\rm gs} \approx 5.5\,L_0$ and at $1/n_{\rm gs} \approx 3.3\,L_0$ for $g\,L_0 = 1.4$. We also observe that the minima are also shifted to larger densities or smaller box sizes and become deeper for larger values of the coupling g. For $g\,L_0 = 0.6$ the minimum is hardly visible on the scale of the plot.

As discussed in Sec. 3.2, it is possible to extract the intrinsic density or the absolute square of the ground-state wavefunction in the center-of-mass frame, see Eqs. (3.52) and (3.53). In Fig. 7.5 we show the results for the dimensionless intrinsic density $|\varphi_2(\bar{r})|^2\,L$ as a function of $\bar{r} = r/L = |x_1 - x_2|/L$ as obtained by the next-to-leading-

[3] The exact continuum-limit results are $E/N|_{\rm cont.} \approx -0.0005\,(1/L_0^2)$ for $g\,L_0 = 0.6$ and $E/N|_{\rm cont.} \approx -0.0024\,(1/L_0^2)$ for $g\,L_0 = 1.0$.

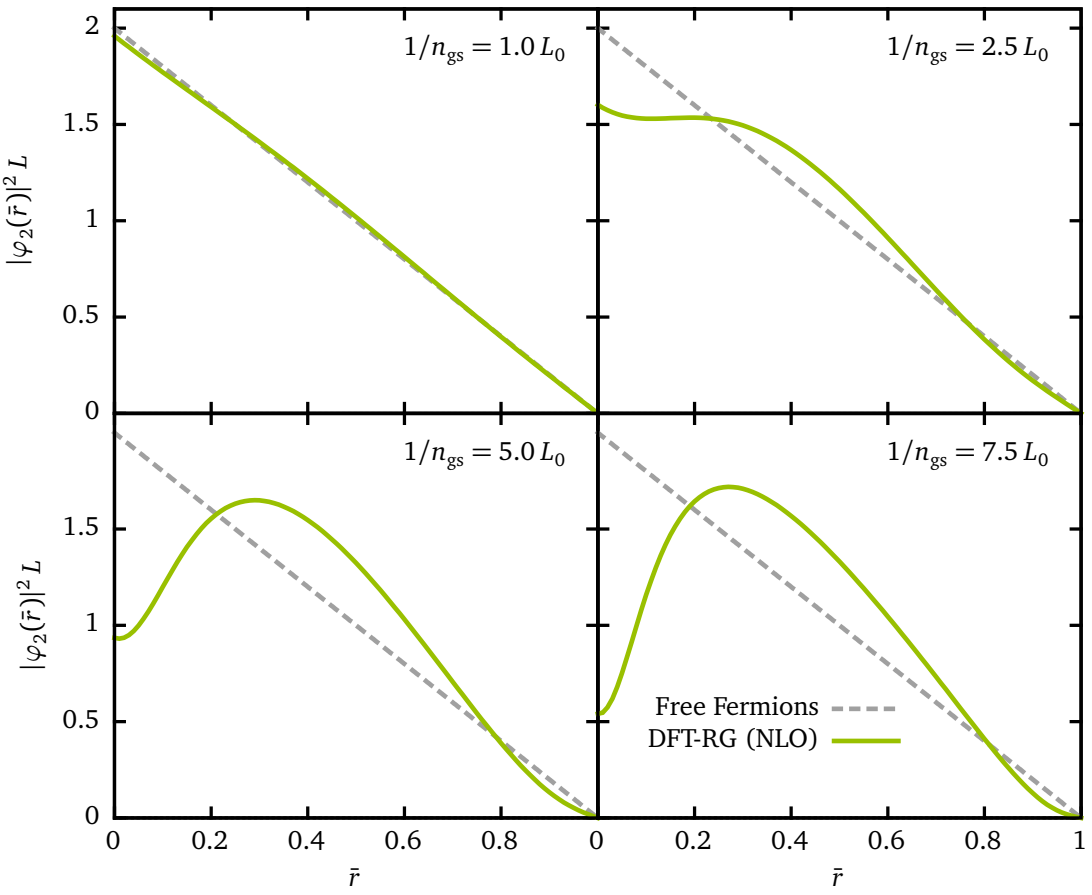

Figure 7.5.: Dimensionless absolute square of the ground-state wavefunction $|\varphi_2(\bar{r})|^2\,L$ in the center-of-mass frame as a function of $\bar{r} = r/L$ as obtained from our DFT-RG approach at next-to-leading order for a coupling constant $g\,L_0 = 0.6$ in comparison with the result for the non-interacting two-body system.

order DFT-RG approximation for a coupling constant of $g\,L_0 = 0.6$ and the result for the non-interaction system of free fermions.

The intrinsic density of the non-interacting system is linear as a function of $\bar{r}$ and the dimensionless quantity $|\varphi_2(\bar{r})|^2\,L = 2(1-\bar{r})$ as a function of $\bar{r}$ does not depend on the ground-state density n_{gs}, whereas our next-to-leading-order DFT-RG result develops a more complex functional form and varies for different ground-state densities n_{gs}. We observe that for larger box sizes the probability of finding the two fermions at the same place decreases. This is due to the short-range repulsive part of the two-body interaction and the fact that the dimensionless coupling $\bar{g}_N$ increases with L. Moreover, we find a maximum in the intrinsic density that appears due to the attractive part of the interaction potential.

Within our DFT-RG framework we are able to treat any combinations of particle numbers $N_\uparrow$ and $N_\downarrow$. After the study of the two-body system, let us now come to systems with higher particle numbers. As a first example we consider systems with one spin-up fermion and different numbers of spin-down fermions. The results for the ground-state energy as a function of the inverse density as obtained by our next-to-leading-order DFT-RG approximation are shown in Fig. 7.6 for various coupling parameters g. For the larger couplings $g\,L_0 = 1.0$ and $g\,L_0 = 1.4$ we observe that the more spin-down particles are in the system the more the value of the density where the zero crossing occures is shifted to lower densities and the minimum becomes less deep or even vanishes. In the case of the smallest coupling we considered in our studies $g\,L_0 = 0.6$ the energies of the systems with more than two fermions are positive in the complete range of the plot. Loosely speaking, since there is no interaction between the particles with identical spin, the spin-down particles only interact with the single spin-up fermion and therefore systems with more spin-down fermions are less bound.

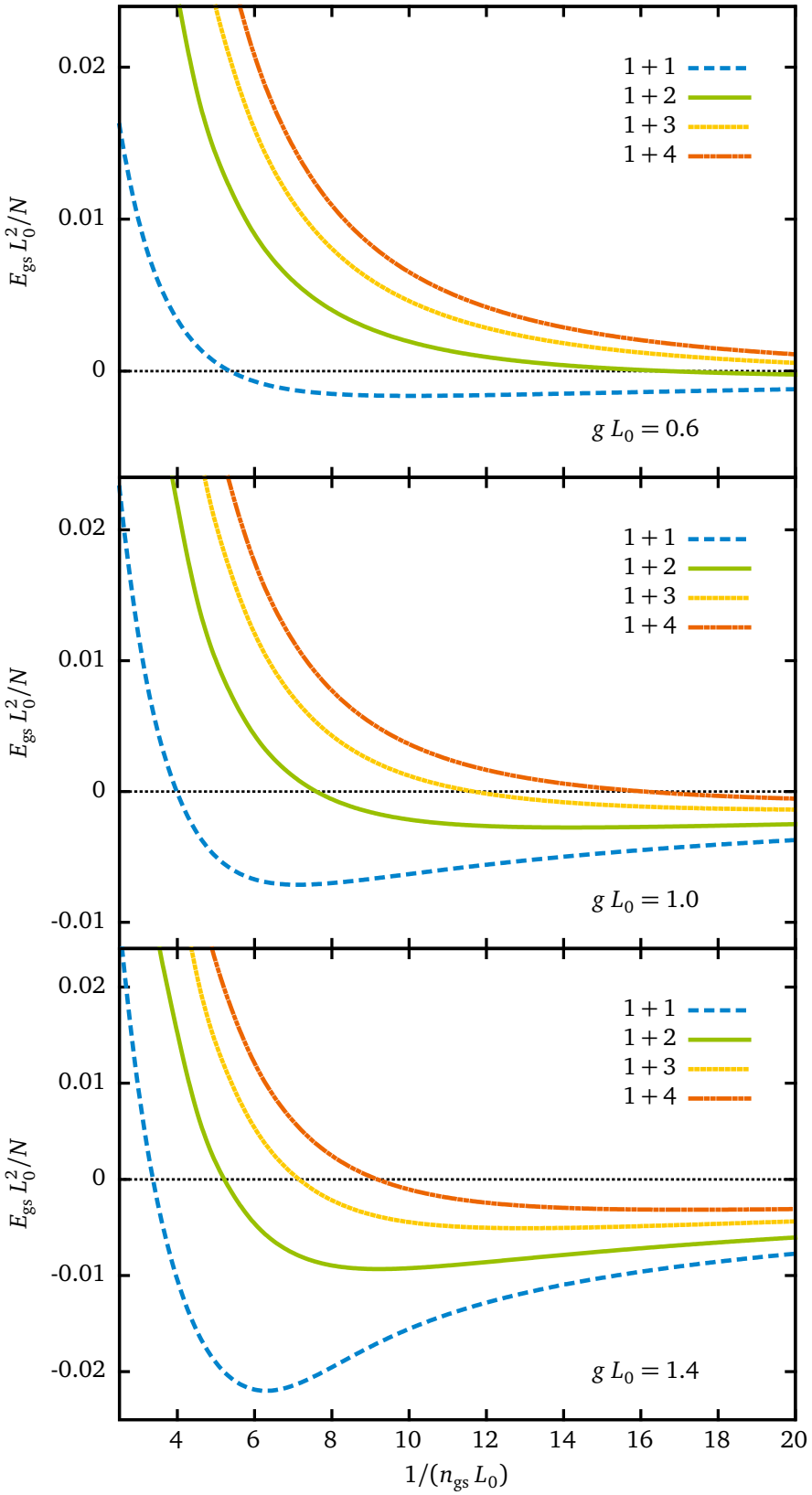

Figure 7.6.: Ground-state energy of systems with different particle numbers as a function of the ground-state density as obtained from our next-to-leading-order DFT-RG approximation. We show the results for one spin-up fermion and different numbers of spin-down fermions.

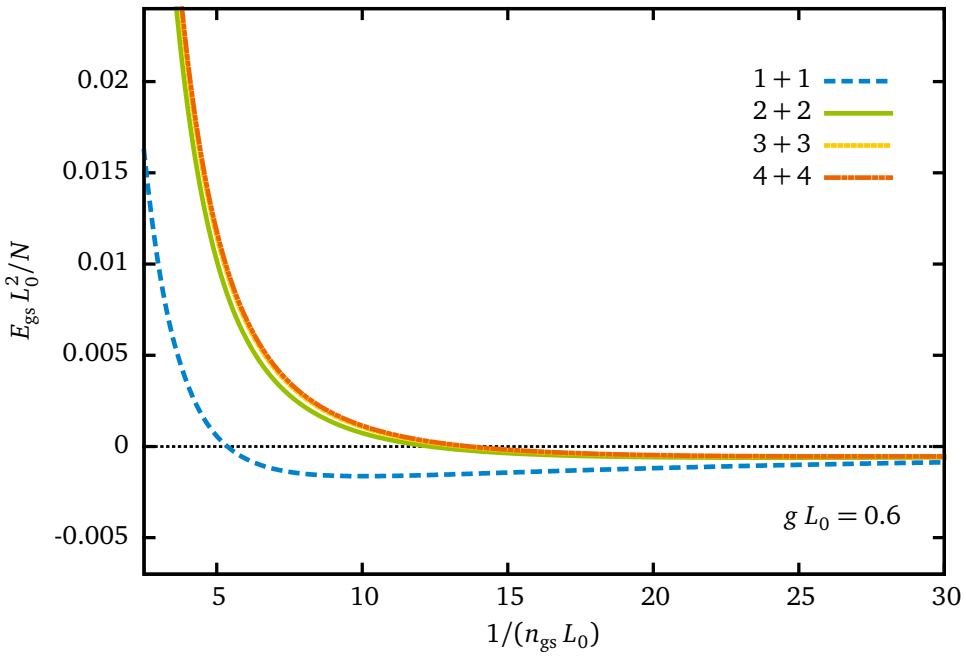

Figure 7.7.: Ground-state energy of systems with different particle numbers as a function of the ground-state density as obtained from our next-to-leading-order DFT-RG approximation. We show the results for equal numbers of spin-up and spin-down fermions.

In Fig. 7.7, we show the ground-state energy as a function of the inverse density n_{gs} for systems with equal numbers of spin-up and spin-down fermions as obtained from our next-to-leading-order DFT-RG approximation. We observe that, our results for the energy per fermion E/N converges rapidly as a function of the fermion number N. In the case of large densities or small box sizes the result for the system with one spin-up and one spin-down fermion deviates significantly from the other results. This may be explained by the fact that in the case of more than two fermions each spin-up fermion interacts with more than just one spin-down fermion and therefore the binding energy is smaller. For large box sizes or small densities these results also line up with the result for the energy per particle of the two-body problem. It seems that there occures a homogenization in the systems if the box is sufficiently large.

Finally, we would like to emphasize again that our approach is not restricted to these two types of systems with higher particle numbers. Within our DFT-RG framework it is in principle possible to study systems with any combination of $N_\uparrow$ spin-up and $N_\downarrow$ spin-down fermions.

7.5 DFT-RG Results – Contact Interaction

In this section, we study systems of spin-$1/2$ fermions interacting via a contact interaction given by

$$U(x_1, x_2) = g\,\delta(x_1 - x_2)\,. \tag{7.51}$$

For positive values of the coupling constant g this is a purely repulsive interaction and for negative values of g the interaction is purely attractive. Also in this case we use the value $L_0 = 0.2$ as a reference length. This length L_0 is no length scale associated with the interaction but for comparison we choose to use the same value here as in the case of the non-local potential.

In Fig. 7.8, we show the ground-state energy per particle as a function of the coupling constant for systems with inverse density $1/n_{gs} = 2.5\,L_0$ as obtained from different approaches, namely the DFT-RG result in leading order

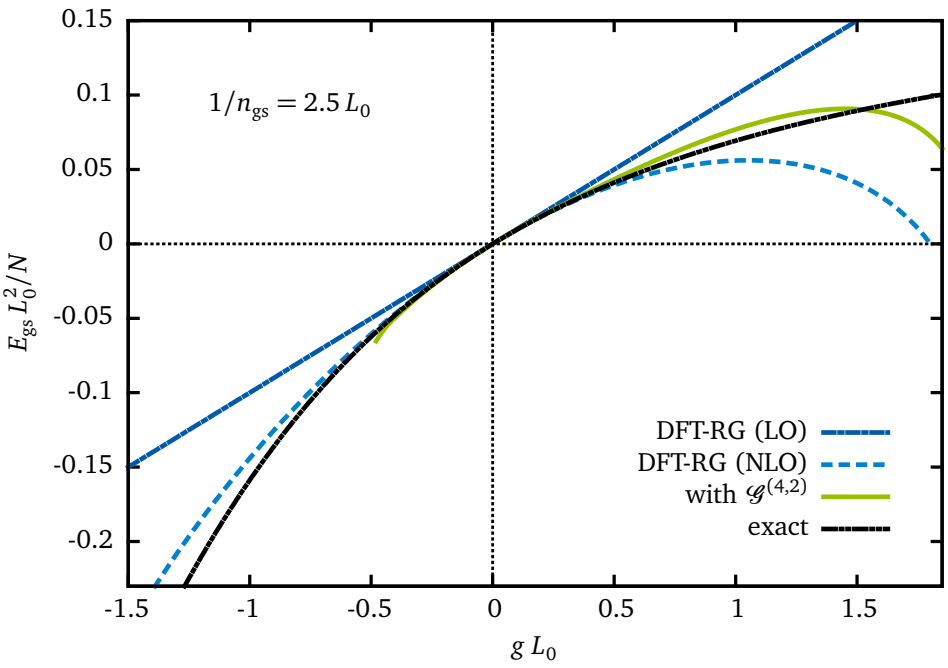

Figure 7.8.: Ground-state energy per particle of the two-body problem with one spin-up and one spin-down fermion as a function of the coupling constant for systems with inverse density $1/n_{gs} = 2.5\,L_0$.

(LO) given by Eq. (7.11), in the next-to-leading-order approximation (NLO) and the improved next-to-leading-order result (with $\mathcal{G}^{(4,2)}$) as discussed in Sec. 7.3. To benchmark our results we also show the exact solution for the ground-state energy as obtained by an analytic calculation of the problem in the center-of-mass frame.[4]

We start with the discussion of purely repulsive interactions. For values of the coupling constant $g > 0$, the two-body system is always unbound. The result obtained by our DFT-RG leading-order approximation is found to be always larger than the exact result and starts to deviate from it at $g\,L_0 \gtrsim 0.2$. At $g\,L_0 \gtrsim 0.5$ also the next-to-leading-order result deviates from the exact result. We observe that the next-to-leading-order result underestimates the exact solution. Since the analytic result for the energy in this approximation shows a singularity, it is not possible to calculate energies for values of the coupling constant larger than $g\,L_0 \gtrsim 1.95$, see our discussion in Sec. 7.3. The improved next-to-leading-order result enhances the range of the coupling where we are able to recover the exact result but the improvement is not able to shift the singularity towards higher couplings.

For purely attractive interactions, where the value of the coupling constant is $g < 0$, the two-body system is always bound. Also in this case the leading-order DFT-RG approximation is always larger than the exact result and starts to deviate from the latter at $g\,L_0 \lesssim -0.2$. The next-to-leading-order result deviates from the exact result at $g\,L_0 \lesssim -0.5$. We observe that the next-to-leading-order result underestimates the absolute value of the exact result also in this case. The improved next-to-leading-order truncation already becomes unstable for values of the coupling constant smaller than $g\,L_0 \lesssim -0.4$.

In Fig. 7.9, we show the ground-state energy per particle as a function of the inverse density as obtained by different approaches. We observe that the result obtained by the leading-order approximation is always greater than the exact result. The upper panel of Fig. 7.9 shows the results for a repulsive interaction with $g\,L_0 = 0.2$. The next-to-leading-order result underestimates the exact result and the improved next-to-leading-order result overestimates the exact ground-state energy. In the lower panel of Fig. 7.9, we show the results for an attractive interaction with $g\,L_0 = -0.2$. The next-to-leading-order result underestimates the exact result and the improved next-to-leading-order result overestimates the absolute value of the exact ground-state energy. Moreover, we observe that

[4] See App. C.3 for the calculation of the exact result of the two-fermion problem.

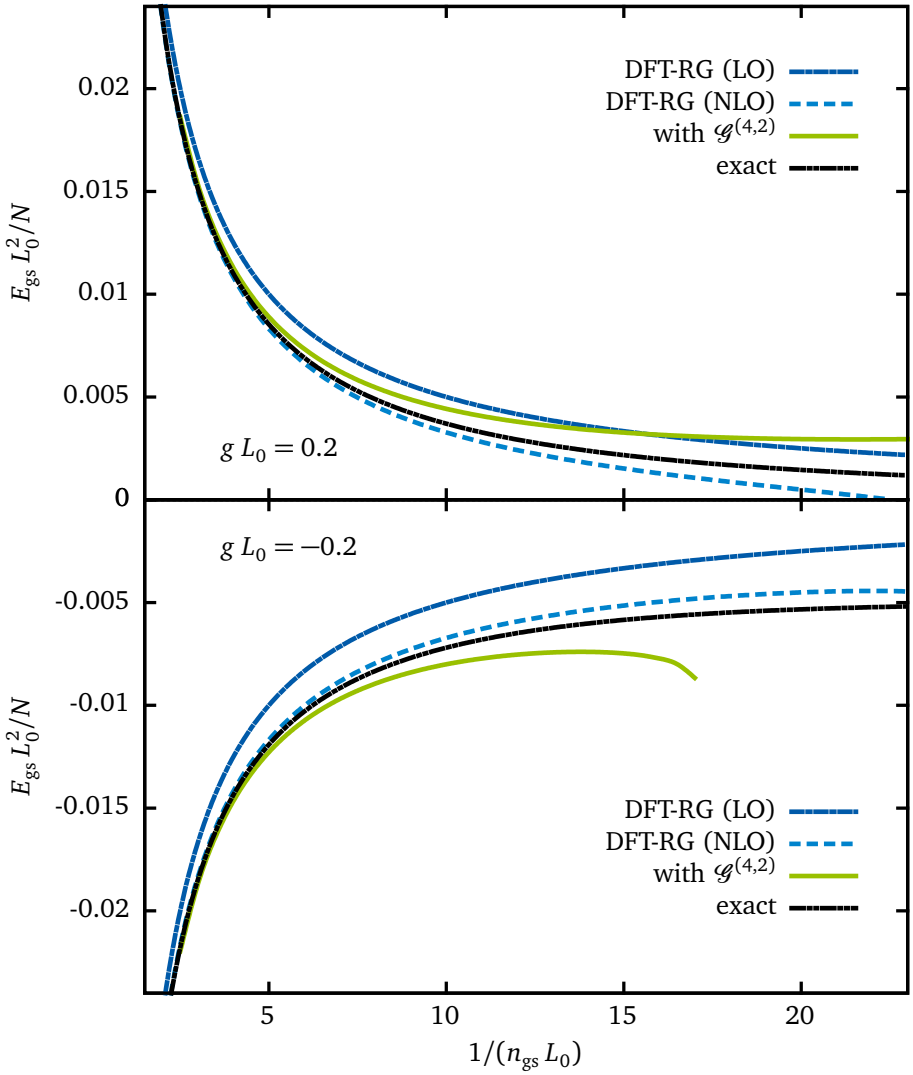

Figure 7.9.: Ground-state energy per particle of the two-body problem with one spin-up and one spin-down fermion as a function of the inverse ground-state density $n_{\rm gs} = N/L$ as obtained by different approaches. Upper panel: Repulsive interaction with $g\,L_0 = 0.2$. Lower panel: Attractive interaction with $g\,L_0 = -0.2$. Note that the ground-state density should not be confused with the intrinsic density of the system.

it is not possible to obtain results for the improved next-to-leading-order result for $1/n_{\rm gs} \gtrsim 17\,L_0$ due to singular behavior of the truncation of the flow equations.

To improve our results further we artificially introduce a factor $(1 + f(g, L)\,\lambda)$ in the term proportional to $\tilde{\mathcal{G}}^{(4,2)}_{\lambda,\uparrow\downarrow,a,a}$ in the flow equation for the up-down-density-density correlation function, see our discussion in Sec. 7.3. Since we already observed that the introduced improvement does not work well in the case of attractive interactions we only study the improvement for the repulsive case here. For convenience we also restrict this study to a fixed value for the coupling constant $g\,L_0 = 0.2$. For the system with one spin-up and one spin-down fermion we adjusted the value of the function $f(g\,L_0 = 0.2, L)$ for various values of L.

These points have then been fitted to a simple linear ansatz

$$f(g = 0.2/L_0, L) = a + b\,L\,, \tag{7.52}$$

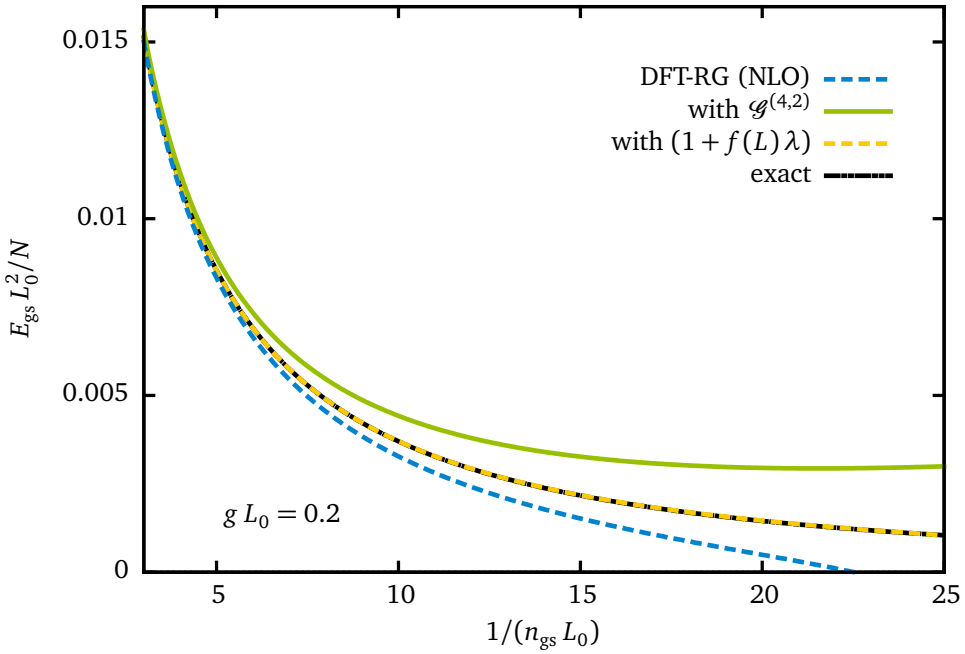

Figure 7.10.: Ground-state energy per particle of the two-body problem with one spin-up and one spin-down fermion as a function of the inverse ground-state density $n_{gs} = N/L$ with a repulsive interaction with $g L_0 = 0.2$. The plot shows the DFT-RG results in next-to-leading-order, the result for the improvement with $\mathcal{G}^{(4,2)}$ and the result obtained by including $f(g, L)$.

where we obtained the results $a = -1.252$ and $b = -0.0102727$ for the two fit parameters. For a fixed value of the coupling constant $g = 0.2/L_0$ we use the replacement

$$\tilde{\mathcal{G}}^{(4,2)}_{\lambda,\uparrow\downarrow,a,a} \quad \rightarrow \quad (1 + (a + b\,L)\,\lambda)\;\tilde{\mathcal{G}}^{(4,2)}_{\lambda,\uparrow\downarrow,a,a} \tag{7.53}$$

in the flow equation for the up-down-density-density correlation function. The result for the ground-state energy obtained with this replacement is shown in Fig 7.10. We observe that it is possible to obtain results that agree identically with the exact result by adjusting the function $f(g, L)$. This suggests that taking the flows of higher-order density correlation functions into account and therefore the λ-dependent density correlation functions of higher orders can cure the problems within the next-to-leading-order approximation. In a next step one could adjust the function $f(g, L)$ over a wider range of the parameters g and L.

In Sec. 3.2, we discussed that it is possible to extract the intrinsic density from the density-density correlation function, see Eqs. (3.52) and (3.53). In Fig. 7.11, we show the results for the dimensionless intrinsic density $|\varphi_2(\bar{r})|^2\, L$ as a function of $\bar{r} = r/L = |x_1 - x_2|/L$ as obtained from the next-to-leading-order DFT-RG approximation for a coupling constant of $g\,L_0 = 0.2$ in the upper panel and of $g\,L_0 = -0.2$ in the lower panel. For comparison we also show the result for the non-interaction system of free fermions.

The intrinsic density of the non-interacting system is linear as a function of $\bar{r}$ and the dimensionless quantity $|\varphi_2(\bar{r})|^2\, L$ is independent of the ground-state density n_{gs}, whereas the intrinsic density of the interacting systems assumes a more complex $\bar{r}$ dependence. For the repulsive interaction we observe that the probability of finding the two fermions at the same place ($\bar{r} = 0$) decreases and for the attractive interaction the probability to find the fermions at the same place increases, as naively expected.

Finally, we discuss our results for systems with higher fermion numbers. We would like to emphasize again that it is in principle possible to study systems with any combination of particle numbers within our DFT-RG framework. We will focus here again on the discussion of two different kinds of many-fermion systems, namely systems with

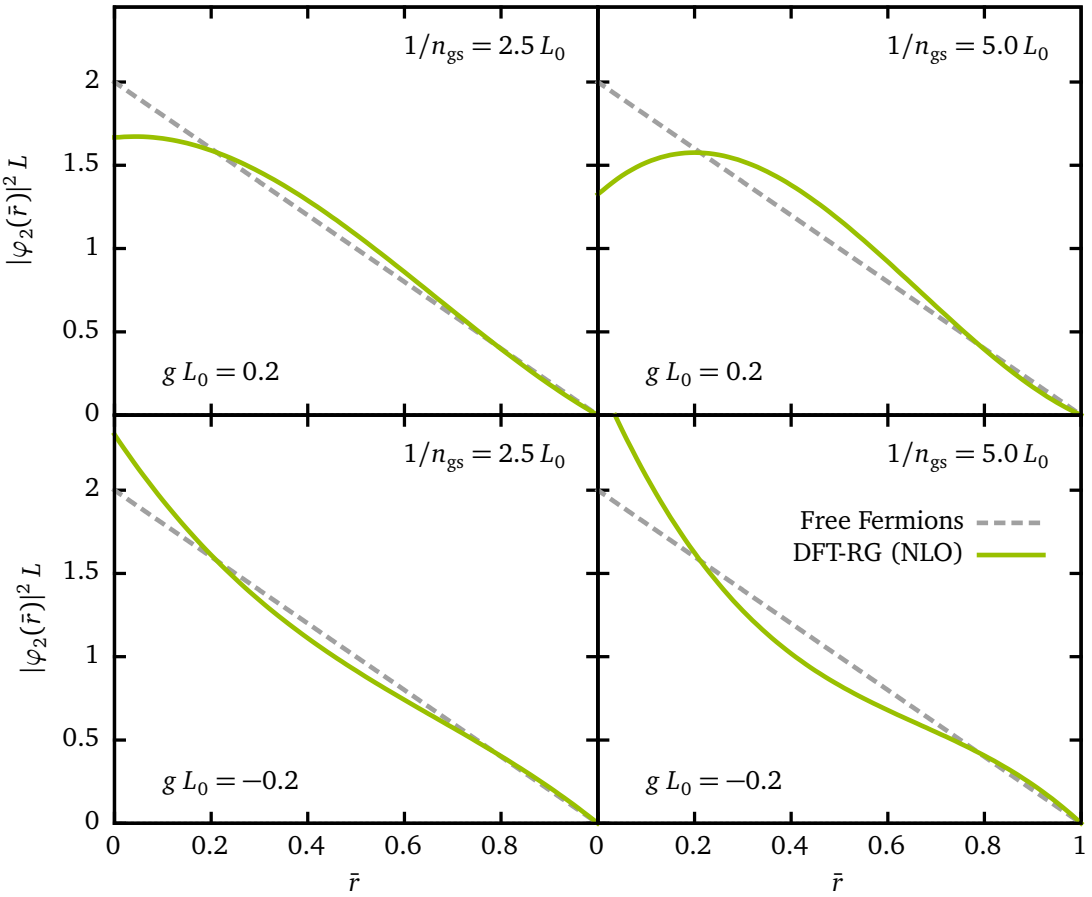

Figure 7.11.: Dimensionless absolute square of the ground-state wavefunction $|\varphi_2(\bar{r})|^2\,L$ in the center-of-mass frame as a function of $\bar{r} = r/L$ as obtained from our DFT-RG approach at NLO in comparison with the result for the non-interacting two-body system. Upper panels: Repulsive interaction with $g\,L_0 = 0.2$. Lower panels: Attractive interaction with $g\,L_0 = -0.2$.

one spin-up fermion and different numbers of spin-down fermions and systems with equal numbers of spin-up and spin-down fermions.

We start with the discussion of systems with one spin-up fermion and $N_\downarrow = 1, 2, 3, 4$ spin-down fermions. In Fig. 7.12, we show the ground-state energy per particle as a function of the inverse ground-state density as obtained from our next-to-leading-order DFT-RG approximation. In the upper panels we show results for a repulsive interaction with $g\,L_0 = 0.2$ and in the lower panels we show results for an attractive interaction with $g\,L_0 = -0.2$.

For the repulsive interaction the energies for all systems are strictly positive. The functional form of all results is qualitatively similar and the energy per particle becomes larger for systems with larger fermion numbers. In the case of the attractive interaction on the other hand the behavior of the systems with more than two fermions deviates significantly from the two-body result. While the ground-state energy of the two-fermion system is negative for small volumes or large densities, the ground-state energies of systems with higher fermion number are positive in this limit. This is due to the fact that in the small-volume limit the kinetic energy associated with the energy of the non-interacting system, $E \sim 1/L^2$, is predominant for the systems with higher particle numbers. The energy of the free two-fermion system is identically zero and therefore the energy in the large-density limit scales as $E \sim g/L$. The zero of E/N shifts to higher values of the inverse density for increasing particle numbers. Since there is no interaction between the particles with identical spin, the spin-down particles only interact with the "impurity" and therefore systems with more spin-down fermions are less bound. This behavior also agrees with our results for the non-local interaction.

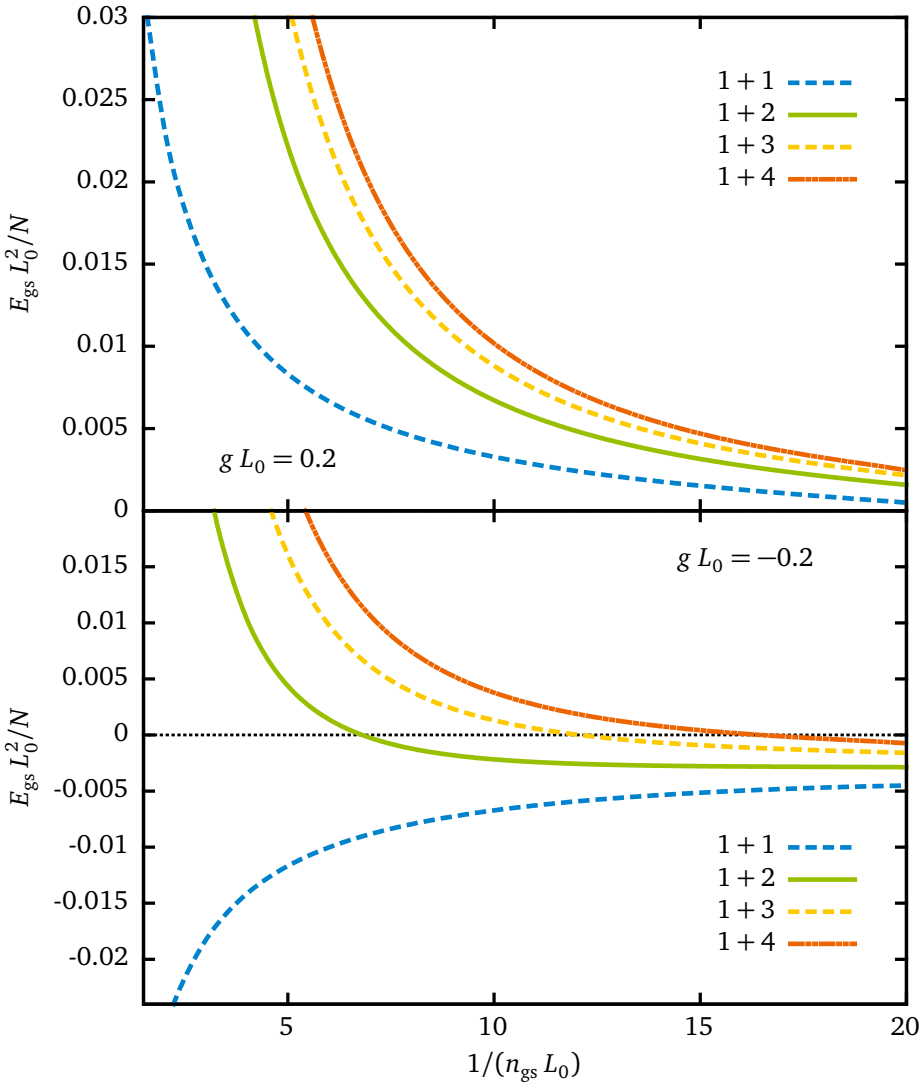

Figure 7.12.: Ground-state energy per particle for systems with one spin-up fermion and different numbers of spin-down fermions as a function of the inverse ground-state density. Upper panel: Repulsive interaction with $g\,L_0 = 0.2$. Lower panel: Attractive interaction with $g\,L_0 = -0.2$.

In Fig. 7.13, we show the ground-state energy as a function of the inverse density n_{gs} for systems with equal numbers of spin-up and spin-down fermions as obtained from our next-to- leading-order DFT-RG approximation. In the upper panel we show the results for a repulsive interaction with $g\,L_0 = 0.2$ and in the lower panel we show the results for an attractive interaction with $g\,L_0 = -0.2$.

We observe that for systems with $N/2 + N/2$ fermions and $N > 2$ the energy per fermion assumes the same value for $1/n_{gs} \gtrsim 12\,L_0$ for the repulsive and the attractive interaction. This agrees also with our finding in the case of the non-local potential. The results for the two-body system differs significantly from the results for the other $N/2 + N/2$ fermion systems over a wide range of the plot. In the case of the attractive potential the energy per particle of the $1 + 1$-fermion system is always negative and approaches its $L \to \infty$ limit from below, whereas the energy per fermion for systems with more particles is positive for small box-sizes or large densities and becomes negative only for $1/n_{gs} \gtrsim 5\,L_0$. This different behavior for the two-body system for small box sizes is due to the fact that the kinetic energy of the two-body system is zero, as discussed above. For large box sizes or small densities the energy per particle of the two-body system agrees with the results for higher particle numbers.

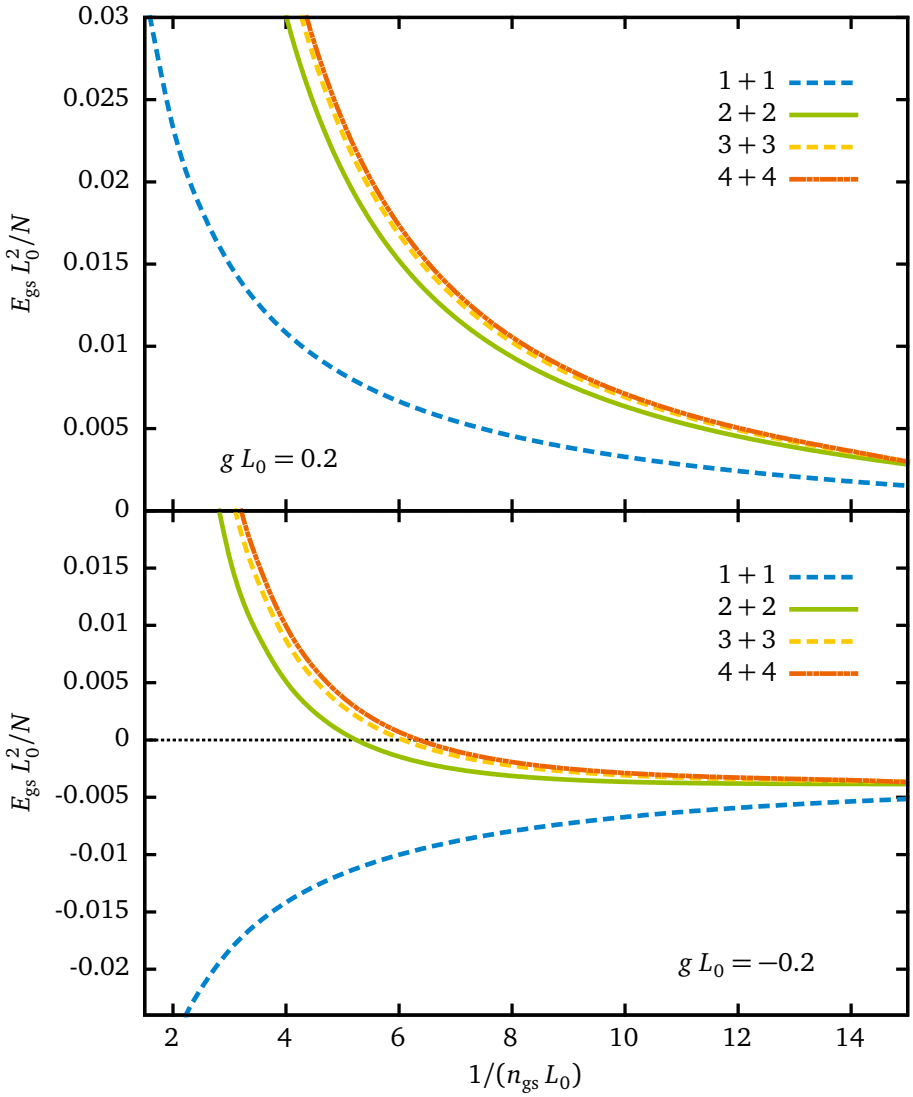

Figure 7.13.: Ground-state energy per particle for systems with equal numbers of spin-up and spin-down fermions as a function of the inverse ground-state density. Upper panel: Repulsive interaction with $g\,L_0 = 0.2$. Lower panel: Attractive interaction with $g\,L_0 = -0.2$.

We would like to mention again that results for all other combinations of spin-up and spin-down fermion numbers can be calculated within our DFT-RG framework. In principle it is also possible to calculate the improved next-to-leading-order result for systems with more than two fermions but we defer the numerical calculation within this approximation to further work.

As a non-trivial observation, we find that E/N converges rapidly as a function of N for both the non-local and the local interaction. Such a rapid convergence is not found in the case of identical fermions. Moreover, an exact result for the N-body problem with a contact interaction yields $E/N \sim N^2$ for large N [71]. This cannot be reproduced with the present truncation whereas for identical fermions our results for E/N are in accordance with *Monte-Carlo* simulations. To improve our result we have to resum all time-independent terms that appear in the perturbative expansion of the up-down-density-density correlation function.

8 Conclusions and Outlook

In this thesis, we have discussed renormalization group techniques to develop an energy density functional from microscopic interactions. In particular, we have derived and discussed an RG flow equation for the energy density functional and applied it for the very first time to physical systems. Still, the focus of our present work is on the conceptional field-theoretical side. Within our approach we have shown that not only ground-state energies, densities as well as the intrinsic density can be computed from the energy density functional but also energies of excited states can be determined rigorously.

Starting from the classical action of a general many-body theory, we derived the 2PPI effective action and argued that the latter can be identified with the density functional. In fact, the 2PPI effective action is a generalization of the *Hohenberg-Kohn* density functional since it contains more information as we have discussed in detail in Sec. 3.6. Our DFT-RG approach relies on an expansion of the energy density functional about the ground-state density rather than a global parametrization of the latter. This expansion is essentially determined by the density-correlation functions from which the absolute square of the wavefunction and excited states can be calculated. We can systematically derive an infinite tower of flow equations for the energy, the density and the density correlation functions within our approach. These RG flow equations allow us to follow the changes of the ground state while the interaction is gradually turned on. The starting point of these differential equations is given by the analytically accessible confined but non-interacting system of free fermions. It is important to introduce such a confining geometry to localize the fermions in this non-interacting limit and fix the particle number, but the choice of the geometry is at our disposal. In this thesis we used a one-dimensional box with (anti)periodic boundary conditions, aiming at the description of ground-state properties of selfbound states in the continuum limit. However, if one aims at the study of other systems one could choose other confining geometries, such as a harmonic trap or a box with "hard walls". Specifically these geometries could be of interest in further studies to describe, e. g., trapped low-dimensional fermion gases with mass- and spin-imbalance which are a good environment to study the transition from few- to many-body systems and are also accessible for experimental studies [28, 29].

An important part of this thesis was to gain a deep insight into the field-theoretical structure of the density functionals and how our DFT-RG framework relates to other methods. Therefore, we discussed the connection between our approach and conventional DFT and how the vertex expansion used in this work is related to the gradient expansion used in other DFT approaches. Moreover, we showed that our approach relates to many-body perturbation theory in a simple and systematic fashion and argued that the coeffients of the perturbative expansion can be extracted from our flow equations. We also discussed the relation of our approach to the *Hartree* and the *Hartree-Fock* approximation. These considerations help to construct meaningful truncation schemes for the in general infinite set of flow equations and guide the construction of density functionals.

As a first step we applied our formalism to a zero-dimensional model to illustrate how our DFT-RG approach works and how ground-state properties can be calculated. In particular, we showed that the results can be systematically improved by taking higher-order n-point functions into account.

We then discussed identical fermions in a one-dimensional nuclear model. We showed that it is possible to extract an upper bound for the ground-state energy in the continuum limit since we found that our results approach the exact result from above in the two-body system. Our continuum-limit approximation in next-to-leading order is already in reasonable agreement with the exact two-body result and with the four- and eight-fermion result obtained by *Monte-Carlo* calculations. In comparison to the exact result of the two-body system we found that our leading-order approximation is off by 40% and our next-to-leading order result deviates still by $\sim 30\%$ from the exact result. Therefore, we shall expect significant contributions from the next higher orders of the density-density

correlation function. Moreover, we could show that within our truncation it is possible to keep spurious fermion self-interactions systematically under control, which often plague density functional approaches.

In the next step, we discussed systems of spin-$1/2$ fermions where only fermions with different spins interact. It is possible to study these systems with any combinations of particle numbers for the spin-up and spin-down fermions and also with different masses. For example, there is no so-called sign problem as in MC calculations which, e. g., hinders the study of spin-imbalance. In this thesis we set the masses of the particles to $m = 1$ for all spin-species, but a generalization to mass-imbalanced systems is straightforward. Once satisfying agreement with, e. g., MC studies in the mass- and spin-balanced case is achieved, this generalization could easily be included in future studies to make predictions for imbalanced systems. The first interaction considered in this system was the same non-local interaction as used in the case of identical fermions. We found that the shape of the results for the energy of the two-body system is qualitatively similar to the one of identical fermions even though the depth of the minimum is larger in the spin-systems. We found that the next-to-leading-order approximation, which also underlied our study of identical fermions, is now plagued by a singular behavior which restricts its application to a finite regime of couplings. For small values of the coupling, this singular behavior is absent for the non-local interaction. To fix this it is neccessary to include higher orders of the density-density correlation function. However, to obtain an approximation for the continuum limit, studies of the convergence behavior of our expansion would be needed. As it is possible with our approach it is possible to describe any combination of fermion numbers for the spin-up and spin-down fermions. We looked at systems with one spin-up fermion and different numbers of spin-down fermions and found that the systems are less bound if we introduce more spin-down fermions in the system. We also looked at systems with equal numbers of spin-up and spin-down fermions and found that the energy per particle saturates for large particle numbers.

Additionally, we discussed systems of spin-$1/2$ fermions interacting via a contact interaction which is a good approximation if one aims at a study of ultracold *Fermi* gases. The breakdown of our next-to-leading-order approximation in terms of the coupling strength can be related to a restriction to finite box sizes for a given g. Therefore, it is impossible to study the continuum-limit behavior of these systems within our present approximations. We find that for finite box sizes our leading-order result is always larger than the exact result and the absolute value of the next-to-leading-order result is smaller. To improve our results we introduced the time-independent term that is missing to recover the third-order perturbative correction of the energy in the flow equation of the up-down-density-density correlation function. Although the obtained results are merely closer to the exact result for strong couplings, we were able to use this constant term to introduce a function depending on the flow parameter λ to estimate a λ-dependent up-down-up-down-density correlation function which is not plagued by a spurious breakdown of the RG flow equations. We indeed showed that it is possible to recover the exact result over a wide range of L by using such a correlation function. This suggests that taking higher-order correlation functions into account fixes the problem with the singular behavior. For this simple feasibility study we included just a time-independent term. However, from our flow equations we see that we have to take the full time dependence of all density correlation functions into account to obtain the exact result if we solve our infinite tower of flow equations. Nevertheless, it is possible to recover the exact continuum-limit result by a resummation of all time-independent terms that appear in the perturbative expansion of the up-down-density-density correlation function [72]. In any case, for systems with higher particle numbers we found similar results for the energy as for the non-local potential within our present approximations. For the system with one spin-up fermion and different numbers of spin-down fermions, the energy per particle increases for increasing numbers of spin-down fermions. In the case of equal numbers of spin-up and spin-down fermions we find that the energy per particle saturates for large fermion numbers, as we also found using the non-local potential. Systems of this type in different confining geometries can be of interest for future study since there are experiments available in low dimensions [28, 29].

We would like to emphasize again that our formalism does not depend on fitting parameters, but is rather a systematic expansion of the energy density functional about the ground-state density. With the recent developments it should now be possible to advance to three-dimensional systems. Since our DFT-RG formalism allows to compute the energy density functional directly from microscopic interactions, it can potentially be used in future studies to

describe realistic nuclei with microscopic interactions derived from chiral effective field theory interactions [17, 73].

Appendices

A Definitions and Abbreviations

In the following we want to list the definitions and abbreviations used throughout this work:

Fourier Transformations

$$f(\tau) = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}\, f(\omega)\, \mathrm{e}^{-\mathrm{i}\omega\tau} \tag{A.1}$$

$$f(\omega) = \int_{-\infty}^{\infty} \mathrm{d}\tau\, f(\tau)\, \mathrm{e}^{\mathrm{i}\omega\tau} \tag{A.2}$$

$$\delta(\tau - \tau') = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}\, \mathrm{e}^{-\mathrm{i}\omega(\tau-\tau')} \tag{A.3}$$

$$2\pi\,\delta(\omega - \omega') = \int_{-\infty}^{\infty} \mathrm{d}\tau\, \mathrm{e}^{\mathrm{i}(\omega-\omega')\tau} \tag{A.4}$$

Fermion Momenta

Here the possible fermion momenta in a box with extend L are given. For odd numbers of fermions we assume periodic boundary conditions:

$$p_k^{(\mathrm{P})} = \frac{2k\,\pi}{L}\,. \tag{A.5}$$

For even numbers of fermions we assume anti-periodic boundary conditions:

$$p_k^{(\mathrm{A})} = \frac{(2k+1)\,\pi}{L}\,. \tag{A.6}$$

One-Particle Energies

Here and in the following is $I_\sigma \in \{\mathrm{P}, \mathrm{A}\}$:

$$\varepsilon_k^{(I_\sigma)} = \frac{1}{2}(p_k^{(I_\sigma)})^2 \tag{A.7}$$

$$\bar{\varepsilon}_{\sigma,k}^{(I_\sigma)} = \varepsilon_k^{(I_\sigma)} - \varepsilon_{\mathrm{F},\sigma}^{(I_\sigma)}\,, \tag{A.8}$$

where the Fermi energies

$$\varepsilon_{\mathrm{F},\sigma}^{(\mathrm{A})} = \varepsilon_{\frac{N_\sigma}{2}-1}^{(\mathrm{A})} \quad (N_\sigma \text{ even}) \quad \text{and} \quad \varepsilon_{\mathrm{F},\sigma}^{(\mathrm{P})} = \varepsilon_{\frac{N_\sigma-1}{2}}^{(\mathrm{P})} \quad (N_\sigma \text{ odd}) \tag{A.9}$$

are determined by the number of spin-σ fermions N_σ.

Some useful relations:

$$\varepsilon_{-k}^{(\mathrm{P})} = \varepsilon_k^{(\mathrm{P})}\,, \tag{A.10}$$

$$\varepsilon_{-k-1}^{(\mathrm{A})} = \varepsilon_k^{(\mathrm{A})} \quad \text{and} \tag{A.11}$$

$$\bar{\varepsilon}_{\sigma,k}^{(I_\sigma)} - \bar{\varepsilon}_{\sigma,l}^{(I_\sigma)} = \varepsilon_k^{(I_\sigma)} - \varepsilon_l^{(I_\sigma)} \tag{A.12}$$

One-Particle Eigenstates

We use plane-wave functions or the eigenfunctions of a box with extend L for our studies in Chaps. 6 and 7,

$$\phi_k^{(I_\sigma)}(x) = \frac{1}{\sqrt{L}}\, \mathrm{e}^{-\mathrm{i}p_k^{(I_\sigma)}x} \tag{A.13}$$

with

$$\int_x (\phi_k^{(I_\sigma)}(x))^* \phi_l^{(I_\sigma)}(x) = \delta_{k,l} \quad \text{and} \tag{A.14}$$

$$\sum_k (\phi_k^{(I_\sigma)}(x_1))^* \phi_k^{(I_\sigma)}(x_2) = \sum_m \delta(x_1 - x_2 + m\,L) \tag{A.15}$$

where $k, l, m \in \mathbb{Z}$.

Some useful relations:

$$\left(\phi_k^{(\mathrm{A})}(x)\right)^* \phi_l^{(\mathrm{A})}(x) = \left(\phi_k^{(\mathrm{P})}(x)\right)^* \phi_l^{(\mathrm{P})}(x) \quad \text{and} \tag{A.16}$$

$$\phi_{-k}^{(\mathrm{P})}(x) = \left(\phi_k^{(\mathrm{P})}(x)\right)^* \tag{A.17}$$

In the thermodynamic limit the momenta p of the fermions become continuous and the associated one-particle wavefunctions are given by

$$\phi_p(x) = \frac{1}{\sqrt{L}}\, \mathrm{e}^{-\mathrm{i}px}\,, \tag{A.18}$$

where the volume-dependent prefactor normalizes these states and the limit $L \to \infty$ is assumed to be taken in the end.

Θ-Functions

The time-like Θ-function is defined in the following way:

$$\Theta_\tau(\tau) = \begin{cases} 1 & \text{for } \tau > 0 \text{ as well as } \tau \to 0^+ \\ 0 & \text{otherwise}\,, \end{cases} \tag{A.19}$$

and the Θ-function for the one-particle energies are:

$$\theta(\pm\bar{\varepsilon}_{\sigma,n}^{(I_\sigma)}) = \begin{cases} 1 & \text{for} \quad \pm\,\bar{\varepsilon}_{\sigma,n}^{(I_\sigma)} \mp \eta > 0\,, \\ 0 & \text{otherwise}\,. \end{cases} \tag{A.20}$$

Here, $\eta \to 0^+$ is tacitly assumed.

Shorthands for Sums, Derivatives and Integrals

The sum over all possible spin states in the system under consideration is given by

$$\sum_\sigma \tag{A.21}$$

and sums with latin indices for systems in a box with periodic boundary conditions:

$$\sum_k = \sum_{k=-\infty}^{\infty} \tag{A.22}$$

Shorthands for derivatives:

$$\partial_\tau = \frac{\partial}{\partial \tau}\,, \qquad \partial_x = \frac{\partial}{\partial x}\,, \qquad \partial_\lambda = \frac{\partial}{\partial \lambda}\,. \tag{A.23}$$

Integrals over τ and ω are always assumed to be as follows:

$$\int_\tau = \int_{-\infty}^{\infty} \mathrm{d}\tau \qquad \text{and} \qquad \int_\omega = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}\,. \tag{A.24}$$

In the case of the spatial integral we distinguish between the general discussion in Chap. 3, where we assume

$$\int_x = \int_{-\infty}^{\infty} \mathrm{d}x \tag{A.25}$$

and the discussion of fermions in a box with extent L, see Chaps. 5, 6 and 7 and Apps. B and C, where we restrict the integration to the domain $[-L/2, L/2)$

$$\int_x = \int_{-L/2}^{L/2} \mathrm{d}x\,. \tag{A.26}$$

B Identical Fermions in a Box

In this appendix we detail the to some extent tedious calculations required to obtain the perturbative corrections for systems of identical fermions. Moreover, we derive the exact result for the two-fermion system.

Since the calculations require rather large expressions we sometimes perform the calculation of additive terms separately. To avoid confusion we would like to mention beforehand that we use the equation number in this chapter mainly to indicate the term we evaluate. In this sense the equation numbers are line numbers indicating an individual line of an equation.

B.1 Leading-Order Perturbative Correction to the Density-Density Correlation Function

Here, we calculate the leading-order perturbative correction to the density-density correlation function $G^{(2)}$. To obtain the latter, the full correlation functions in Eq. (5.25) are replaced by their zeroth-order expansion coefficient, i. e. $G^{(2)}_\lambda \to G^{(2)}_{\lambda=0} \equiv G^{(2,0)}$ and $G^{(4)}_\lambda \to G^{(4)}_{\lambda=0} \equiv G^{(4,0)}$. The flow equation for $G^{(2,1)}_\lambda$ then reads:

$$\begin{aligned}\partial_\lambda G^{(2,1)}_\lambda(\tau_1,x_1,\tau_2,x_2) =& -\frac{N}{L}\int_{\tau_3}\int_{x_3}\int_{x_4} G^{(2,0)}(\tau_1,x_1,\tau_3,x_3)\,\mathfrak{U}(x_3-x_4)\,G^{(2,0)}(\tau_3,x_4,\tau_2,x_2)\\ &-\frac{N}{2L}\int_{\tau_3}\int_{x_3}\int_{x_4}\mathfrak{U}(x_3-x_4)\,G^{(4,0)}(\tau_3,x_4,\tau_3,x_3,\tau_1,x_1,\tau_2,x_2)\\ =& -\frac{N}{L}\left(\mathscr{G}^{(2,1)}(\tau_1,x_1,\tau_2,x_2)+\mathscr{G}^{(4,1)}(\tau_1,x_1,\tau_2,x_2)\right). \end{aligned} \tag{B.1}$$

We named the first term $\mathscr{G}^{(2,1)}$ and the second term $\mathscr{G}^{(4,1)}$ so that we can calculate them separately to avoid confusion. We start to evaluate the first term by using Eqs. (5.5) and (5.6) and the definition of $G^{(2)}_{\lambda=0}$ given in Eq. (3.28):

$$\begin{aligned}&\mathscr{G}^{(2,1)}(\tau_1,x_1,\tau_2,x_2)\\ &\quad=\int_{\tau_3}\int_{x_3}\int_{x_4} G^{(2,0)}(\tau_1,x_1,\tau_3,x_3)\,\mathfrak{U}(x_3-x_4)\,G^{(2,0)}(\tau_3,x_4,\tau_2,x_2)\\ &\quad=\int_{\tau_3}\int_{x_3}\int_{x_4} G^{(2,0)}(\tau_1,x_1,\tau_3,x_3)\sum_m \mathfrak{U}_{m,m}\,(\phi^{(\mathrm{P})}_m(x_3))^*\phi^{(\mathrm{P})}_m(x_4)\,G^{(2,0)}(\tau_3,x_4,\tau_2,x_2)\\ &\quad=\int_{\tau_3}\int_{x_3}\int_{x_4}\sum_m \mathfrak{U}_{m,m}\,(\phi^{(\mathrm{P})}_m(x_3))^*\phi^{(\mathrm{P})}_m(x_4)\,\Delta^{(I)}_{\lambda=0}(\tau_1,x_1,\tau_3,x_3)\,\Delta^{(I)}_{\lambda=0}(\tau_3,x_3,\tau_1,x_1)\\ &\qquad\qquad\qquad

$$
\begin{aligned}
&= \sum_m \mathfrak{U}_{m,m} \sum_{k_1 \dots k_4} \int_{\omega_1} \cdots \int_{\omega_4} \left(-\mathrm{i}\,\omega_1 + \bar{\varepsilon}^{(I)}_{k_1}\right)^{-1} \left(-\mathrm{i}\,\omega_2 + \bar{\varepsilon}^{(I)}_{k_2}\right)^{-1} \left(-\mathrm{i}\,\omega_3 + \bar{\varepsilon}^{(I)}_{k_3}\right)^{-1} \left(-\mathrm{i}\,\omega_4 + \bar{\varepsilon}^{(I)}_{k_4}\right)^{-1} \\
&\qquad \frac{\delta_{k_2+m,k_1}}{\sqrt{L}} \frac{\delta_{k_4+m,k_3}}{\sqrt{L}}\, 2\pi\,\delta(\omega_1 - \omega_2 - \omega_3 + \omega_4) \\
&\qquad\quad \mathrm{e}^{-\mathrm{i}\,\omega_1 \tau_1} \mathrm{e}^{\mathrm{i}\,\omega_2 \tau_1} \mathrm{e}^{\mathrm{i}\,\omega_3 \tau_2} \mathrm{e}^{-\mathrm{i}\,\omega_4 \tau_2}\, (\phi^{(\mathrm{P})}_{k_1}(x_1))^* \, \phi^{(\mathrm{P})}_{k_2}(x_1)\, \phi^{(\mathrm{P})}_{k_3}(x_2) (\phi^{(\mathrm{P})}_{k_4}(x_2))^* \\
&= \frac{1}{L} \sum_m \mathfrak{U}_{m,m} \sum_{k,l} \int_{\omega_1} \int_{\omega_2} \int_{\omega_3} \left(-\mathrm{i}\,\omega_1 + \bar{\varepsilon}^{(I)}_{k+m}\right)^{-1} \left(-\mathrm{i}\,\omega_2 + \bar{\varepsilon}^{(I)}_{k}\right)^{-1} \left(-\mathrm{i}\,\omega_3 + \bar{\varepsilon}^{(I)}_{l+m}\right)^{-1} \left(\mathrm{i}(\omega_1 - \omega_2 - \omega_3) + \bar{\varepsilon}^{(I)}_{l}\right)^{-1} \\
&\qquad \mathrm{e}^{-\mathrm{i}\,\omega_1 \tau_1} \mathrm{e}^{\mathrm{i}\,\omega_2 \tau_1} \mathrm{e}^{\mathrm{i}\,\omega_3 \tau_2} \mathrm{e}^{-\mathrm{i}(\omega_1 - \omega_2 - \omega_3), \tau_2}\, (\phi^{(\mathrm{P})}_{k+m}(x_1))^* \, \phi^{(\mathrm{P})}_{k}(x_1)\, \phi^{(\mathrm{P})}_{l+m}(x_2) (\phi^{(\mathrm{P})}_{l}(x_2))^* \\
&= \frac{1}{L^2} \sum_m \mathfrak{U}_{m,m} \sum_{k,l} \int_{\omega_1} \int_{\omega_2} \int_{\omega_3} \left(-\mathrm{i}\,\omega_1 + \bar{\varepsilon}^{(I)}_{k+m}\right)^{-1} \left(-\mathrm{i}\,\omega_2 + \bar{\varepsilon}^{(I)}_{k}\right)^{-1} \left(-\mathrm{i}\,\omega_3 + \bar{\varepsilon}^{(I)}_{l+m}\right)^{-1} \left(\mathrm{i}(\omega_1 - \omega_2 - \omega_3) + \bar{\varepsilon}^{(I)}_{l}\right)^{-1} \\
&\qquad \mathrm{e}^{-\mathrm{i}\,\omega_1 (\tau_1 - \tau_2)} \mathrm{e}^{-\mathrm{i}\,\omega_2 (\tau_2 - \tau_1)}\, (\phi^{(\mathrm{P})}_{m}(x_1))^* \, \phi^{(\mathrm{P})}_{m}(x_2), \qquad \text{(B.2)}
\end{aligned}
$$

where we plugged in the definition for $\Delta^{(I)}_{\lambda=0}$ given in Eq. (5.11) and introduced the shorthand $\int_\omega = \int_{-\infty}^{\infty} \frac{\mathrm{d}\omega}{2\pi}$. We also used the relation $(\phi^{(\mathrm{A})}_k(x))^* \phi^{(\mathrm{A})}_l(x) = (\phi^{(\mathrm{P})}_k(x))^* \phi^{(\mathrm{P})}_l(x)$ for the anti-periodic one-particle eigenstates.

Now we will start to evaluate the ω integrals:

$$
\begin{aligned}
&\mathscr{G}^{(2,1)}(\tau_1, x_1, \tau_2, x_2) \\
&\quad = \frac{1}{L^2} \sum_m \mathfrak{U}_{m,m} \sum_{k,l} \int_{\omega_1} \int_{\omega_2} \left(-\mathrm{i}\,\omega_1 + \bar{\varepsilon}^{(I)}_{k+m}\right)^{-1} \left(-\mathrm{i}\,\omega_2 + \bar{\varepsilon}^{(I)}_{k}\right)^{-1} \left(\mathrm{i}(\omega_1 - \omega_2) + \bar{\varepsilon}^{(I)}_{l} - \bar{\varepsilon}^{(I)}_{l+m}\right)^{-1} \\
&\qquad \left(\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l}) - \Theta(-\bar{\varepsilon}^{(I)}_{l+m})\Theta(\bar{\varepsilon}^{(I)}_{l})\right) \mathrm{e}^{-\mathrm{i}\,\omega_1 (\tau_1 - \tau_2)} \mathrm{e}^{-\mathrm{i}\,\omega_2 (\tau_2 - \tau_1)}\, (\phi^{(\mathrm{P})}_{m}(x_1))^* \, \phi^{(\mathrm{P})}_{m}(x_2) \\
&\quad = \frac{1}{L^2} \sum_{m \neq 0} \mathfrak{U}_{m,m} \sum_{k,l} \int_{\omega_1} \left(-\mathrm{i}\,\omega_1 + \bar{\varepsilon}^{(I)}_{k+m}\right)^{-1} \left(-\mathrm{i}\,\omega_1 + \bar{\varepsilon}^{(I)}_{k} - \bar{\varepsilon}^{(I)}_{l} + \bar{\varepsilon}^{(I)}_{l+m}\right)^{-1} \mathrm{e}^{-\mathrm{i}\,\omega_1 (\tau_1 - \tau_2)} \\
&\qquad \Big\{ -\mathrm{e}^{(\bar{\varepsilon}^{(I)}_{l} - \bar{\varepsilon}^{(I)}_{l+m})(\tau_1 - \tau_2)} \mathrm{e}^{-\mathrm{i}\,\omega_1 (\tau_1 - \tau_2)} \left(\Theta_\tau(\tau_1 - \tau_2)\Theta(-\bar{\varepsilon}^{(I)}_{l} + \bar{\varepsilon}^{(I)}_{l+m}) - \Theta_\tau(\tau_2 - \tau_1)\Theta(\bar{\varepsilon}^{(I)}_{l} - \bar{\varepsilon}^{(I)}_{l+m})\right) \\
&\qquad\quad + \mathrm{e}^{\bar{\varepsilon}^{(I)}_{k}(\tau_1 - \tau_2)} \left(\Theta_\tau(\tau_1 - \tau_2)\Theta(\bar{\varepsilon}^{(I)}_{k}) - \Theta_\tau(\tau_2 - \tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{k})\right) \Big\} \\
&\qquad \left(\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l}) - \Theta(-\bar{\varepsilon}^{(I)}_{l+m})\Theta(\bar{\varepsilon}^{(I)}_{l})\right)\, (\phi^{(\mathrm{P})}_{m}(x_1))^* \, \phi^{(\mathrm{P})}_{m}(x_2) \\
&\quad = \frac{1}{L^2} \sum_{m \neq 0} \mathfrak{U}_{m,m} \sum_{k,l} \int_{\omega_1} \left(-\mathrm{i}\,\omega_1 + \bar{\varepsilon}^{(I)}_{k+m}\right)^{-1} \left(-\mathrm{i}\,\omega_1 + \bar{\varepsilon}^{(I)}_{k} - \bar{\varepsilon}^{(I)}_{l} + \bar{\varepsilon}^{(I)}_{l+m}\right)^{-1} \mathrm{e}^{-\mathrm{i}\,\omega_1 (\tau_1 - \tau_2)} \\
&\qquad \left(\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l}) - \Theta(-\bar{\varepsilon}^{(I)}_{l+m})\Theta(\bar{\varepsilon}^{(I)}_{l})\right)\, (\phi^{(\mathrm{P})}_{m}(x_1))^* \, \phi^{(\mathrm{P})}_{m}(x_2) \\
&\qquad \Big\{ -\mathrm{e}^{(\bar{\varepsilon}^{(I)}_{l} - \bar{\varepsilon}^{(I)}_{l+m})(\tau_1 - \tau_2)} \mathrm{e}^{-\mathrm{i}\,\omega_1 (\tau_1 - \tau_2)} \left(\Theta_\tau(\tau_1 - \tau_2)\Theta(-\bar{\varepsilon}^{(I)}_{l} + \bar{\varepsilon}^{(I)}_{l+m}) - \Theta_\tau(\tau_2 - \tau_1)\Theta(\bar{\varepsilon}^{(I)}_{l} - \bar{\varepsilon}^{(I)}_{l+m})\right) \qquad \text{(B.3)} \\
&\qquad\quad + \mathrm{e}^{\bar{\varepsilon}^{(I)}_{k}(\tau_1 - \tau_2)} \left(\Theta_\tau(\tau_1 - \tau_2)\Theta(-\bar{\varepsilon}^{(I)}_{k}) - \Theta_\tau(\tau_2 - \tau_1)\Theta(\bar{\varepsilon}^{(I)}_{k})\right) \Big\}, \qquad \text{(B.4)}
\end{aligned}
$$

where we excluded the term with $m = 0$ in the sum because $\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l}) - \Theta(-\bar{\varepsilon}^{(I)}_{l+m})\Theta(\bar{\varepsilon}^{(I)}_{l})$ is equal to zero for $m = 0$. Note that we use the equation numbers (B.3) and (B.4) to intricate the two additive terms appearing in the calculation of $\mathscr{G}^{(2,1)}$. We use this below to indicate which of the terms we evaluate. Before we go on with the evaluation of $\mathscr{G}^{(2,1)}$, we want to take a closer look at the terms of the Θ-functions and find the following relations:

$$
\begin{aligned}
\Theta(\bar{\varepsilon}^{(I)}_{k} - \bar{\varepsilon}^{(I)}_{l})\Theta(\bar{\varepsilon}^{(I)}_{k})\Theta(-\bar{\varepsilon}^{(I)}_{l}) &= \Theta(\bar{\varepsilon}^{(I)}_{k})\Theta(-\bar{\varepsilon}^{(I)}_{l}) \\
\Theta(\bar{\varepsilon}^{(I)}_{k} - \bar{\varepsilon}^{(I)}_{l})\Theta(-\bar{\varepsilon}^{(I)}_{k})\Theta(\bar{\varepsilon}^{(I)}_{l}) &= 0\,.
\end{aligned} \qquad \text{(B.5)}
$$

With these we can simplify the Θ-terms apearing in line (B.3):

$$
\begin{aligned}
&\left(\Theta_\tau(\tau_1 - \tau_2)\Theta(-\bar{\varepsilon}^{(I)}_{l} + \bar{\varepsilon}^{(I)}_{l+m}) - \Theta_\tau(\tau_2 - \tau_1)\Theta(\bar{\varepsilon}^{(I)}_{l} - \bar{\varepsilon}^{(I)}_{l+m})\right) \left(\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l}) - \Theta(-\bar{\varepsilon}^{(I)}_{l+m})\Theta(\bar{\varepsilon}^{(I)}_{l})\right) \\
&= \Theta_\tau(\tau_1 - \tau_2)\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l}) + \Theta_\tau(\tau_2 - \tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{l+m})\Theta(\bar{\varepsilon}^{(I)}_{l}), \qquad \text{(B.6)}
\end{aligned}
$$

and use this in the evaluation of line (B.3):

$$
\begin{aligned}
&-\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\int_{\omega_1}\left(-\mathrm{i}\,\omega_1+\bar{\varepsilon}^{(I)}_{k+m}\right)^{-1}\left(-\mathrm{i}\,\omega_1+\bar{\varepsilon}^{(I)}_{k}-\bar{\varepsilon}^{(I)}_{l}+\bar{\varepsilon}^{(I)}_{l+m}\right)^{-1}\,\mathrm{e}^{(\bar{\varepsilon}^{(I)}_{l}-\bar{\varepsilon}^{(I)}_{l+m})(\tau_1-\tau_2)}\\
&\qquad\left(\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l})+\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{l+m})\Theta(\bar{\varepsilon}^{(I)}_{l})\right)\,(\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
=&-\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\left(\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l}\right)^{-1}\,\mathrm{e}^{(\bar{\varepsilon}^{(I)}_{l}-\bar{\varepsilon}^{(I)}_{l+m})(\tau_1-\tau_2)}\,(\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\left(\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l})+\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{l+m})\Theta(\bar{\varepsilon}^{(I)}_{l})\right)\\
&\qquad\quad\left(\Theta(-\bar{\varepsilon}^{(I)}_{k+m})\Theta(\bar{\varepsilon}^{(I)}_{l+m}+\bar{\varepsilon}^{(I)}_{k}-\bar{\varepsilon}^{(I)}_{l})-\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l})\right)\\
=&-\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\left(\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l}\right)^{-1}\,\mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{l}-\bar{\varepsilon}^{(I)}_{l+m}||\tau_1-\tau_2|}\,(\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\Big\{\;\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l})\,\left(\Theta(\bar{\varepsilon}^{(I)}_{l+m}+\bar{\varepsilon}^{(I)}_{k}-\bar{\varepsilon}^{(I)}_{l})-\Theta(\bar{\varepsilon}^{(I)}_{k+m})\right)\\
&\qquad+\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{l+m})\Theta(\bar{\varepsilon}^{(I)}_{l})\,\left(\Theta(-\bar{\varepsilon}^{(I)}_{k+m})-\Theta(-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l})\right)\Big\}\,.
\end{aligned}
\tag{B.7}
$$

We excluded the term with $k=l$ in the sums here because for this term the ω_1 integral reduces to

$$
\int\frac{\mathrm{d}\omega_1}{2\pi}\,\left(-\mathrm{i}\,\omega_1+\bar{\varepsilon}^{(I)}_{k+m}\right)^{-2}=0\,,
\tag{B.8}
$$

and used the following relation for the Θ-functions:

$$
\Theta(a)\Theta(b)-\Theta(-a)\Theta(-b)=\Theta(a)-\Theta(-b)\,.
\tag{B.9}
$$

The latter can be used to simplify the Θ-terms in two ways:

$$
\begin{aligned}
&\Theta(-\bar{\varepsilon}^{(I)}_{k+m})\Theta(\bar{\varepsilon}^{(I)}_{l+m}+\bar{\varepsilon}^{(I)}_{k}-\bar{\varepsilon}^{(I)}_{l})-\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l})=\Theta(\bar{\varepsilon}^{(I)}_{l+m}+\bar{\varepsilon}^{(I)}_{k}-\bar{\varepsilon}^{(I)}_{l})-\Theta(\bar{\varepsilon}^{(I)}_{k+m})\,,\\
&\Theta(-\bar{\varepsilon}^{(I)}_{k+m})\Theta(\bar{\varepsilon}^{(I)}_{l+m}+\bar{\varepsilon}^{(I)}_{k}-\bar{\varepsilon}^{(I)}_{l})-\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l})=\Theta(-\bar{\varepsilon}^{(I)}_{k+m})-\Theta(-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l})\,.
\end{aligned}
\tag{B.10}
$$

It will become clear why we choose to use these two different transformations when we further simplify our results.

In the second line (B.4) it is in particular important to look at the $k=l$ term seperately:

$$
\begin{aligned}
&\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k}\int_{\omega_1}\left(-\mathrm{i}\,\omega_1+\bar{\varepsilon}^{(I)}_{k+m}\right)^{-2}\,\mathrm{e}^{-\mathrm{i}\,\omega_1(\tau_1-\tau_2)}\,\mathrm{e}^{\bar{\varepsilon}^{(I)}_{k}(\tau_1-\tau_2)}\,(\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\left(\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_{k})-\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{k+m})\Theta(\bar{\varepsilon}^{(I)}_{k})\right)\\
=&\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k}\,\mathrm{e}^{\bar{\varepsilon}^{(I)}_{k}(\tau_1-\tau_2)}\,(\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\mathrm{e}^{-\bar{\varepsilon}^{(I)}_{k+m}(\tau_1-\tau_2)}(\tau_1-\tau_2)\left(\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_{k+m})-\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{k+m})\right)\\
&\qquad\left(\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_{k})-\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{k+m})\Theta(\bar{\varepsilon}^{(I)}_{k})\right)\\
=&\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k}\,\mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_{k}||\tau_1-\tau_2|}\,|\tau_1-\tau_2|\,(\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\left(\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_{k})+\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{k+m})\Theta(\bar{\varepsilon}^{(I)}_{k})\right)\\
=&\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k}\,\mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_{k}||\tau_1-\tau_2|}\,|\tau_1-\tau_2|\,\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_{k})\,(\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\,,
\end{aligned}
\tag{B.11}
$$

where we shifted the sum for the term depending on $\Theta_\tau(\tau_2-\tau_1)$ in the last step. For odd particle numbers or $I=\mathrm{P}$ the shift is $k\to -k-m$ and for even particle numbers or $I=\mathrm{A}$ the shift is $k\to -k-m-1$. We can then use

$$\begin{aligned}\bar{\varepsilon}_k^{(\mathrm{P})} &= \bar{\varepsilon}_{-k}^{(\mathrm{P})} \quad \text{and}\\ \bar{\varepsilon}_k^{(\mathrm{A})} &= \bar{\varepsilon}_{-k-1}^{(\mathrm{A})}\end{aligned} \tag{B.12}$$

to remove the $\Theta_\tau(\tau)$-functions here.

Now we come back to the evaluation of all other terms, namely the ones with $k\neq l$, in the second line (B.4):

$$\begin{aligned}&\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\int_{\omega_1}\left(-\mathrm{i}\,\omega_1+\bar{\varepsilon}_{k+m}^{(I)}\right)^{-1}\left(-\mathrm{i}\,\omega_1+\bar{\varepsilon}_k^{(I)}-\bar{\varepsilon}_l^{(I)}+\bar{\varepsilon}_{l+m}^{(I)}\right)^{-1}\mathrm{e}^{-\mathrm{i}\,\omega_1(\tau_1-\tau_2)}\,\mathrm{e}^{\bar{\varepsilon}_k^{(I)}(\tau_1-\tau_2)}\,(\phi_m^{(\mathrm{P})}(x_1))^*\,\phi_m^{(\mathrm{P})}(x_2)\\ &\qquad\left(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar{\varepsilon}_k^{(I)})-\Theta_\tau(\tau_2-\tau_1)\Theta(\bar{\varepsilon}_k^{(I)})\right)\left(\Theta(\bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_l^{(I)})-\Theta(-\bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_l^{(I)})\right)\\ =&\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\left(\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_k^{(I)}+\bar{\varepsilon}_l^{(I)}\right)^{-1}\mathrm{e}^{\bar{\varepsilon}_k^{(I)}(\tau_1-\tau_2)}\,(\phi_m^{(\mathrm{P})}(x_1))^*\,\phi_m^{(\mathrm{P})}(x_2)\\ &\qquad\left(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar{\varepsilon}_k^{(I)})-\Theta_\tau(\tau_2-\tau_1)\Theta(\bar{\varepsilon}_k^{(I)})\right)\left(\Theta(\bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_l^{(I)})-\Theta(-\bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_l^{(I)})\right)\\ &\qquad\Big\{-\mathrm{e}^{-\bar{\varepsilon}_{k+m}^{(I)}(\tau_1-\tau_2)}\left(\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}_{k+m}^{(I)})-\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}_{k+m}^{(I)})\right) \qquad\text{(B.13)}\\ &\qquad+\mathrm{e}^{(-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_k^{(I)}+\bar{\varepsilon}_l^{(I)})(\tau_1-\tau_2)}\left(\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}_{l+m}^{(I)}+\bar{\varepsilon}_k^{(I)}-\bar{\varepsilon}_l^{(I)})-\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_k^{(I)}+\epsilon_l)\right)\Big\}. \qquad\text{(B.14)}\end{aligned}$$

We can simplify the first line (B.13):

$$\begin{aligned}&-\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\left(\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_k^{(I)}+\bar{\varepsilon}_l^{(I)}\right)^{-1}\mathrm{e}^{-|\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_k^{(I)}||\tau_1-\tau_2|}\,(\phi_m^{(\mathrm{P})}(x_1))^*\,\phi_m^{(\mathrm{P})}(x_2)\\ &\qquad\Big(\ \Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}_{k+m}^{(I)})\Theta(-\bar{\varepsilon}_k^{(I)})\left(\Theta(\bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_l^{(I)})-\Theta(-\bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_l^{(I)})\right)\\ &\qquad+\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}_{k+m}^{(I)})\Theta(\bar{\varepsilon}_k^{(I)})\left(\Theta(\bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_l^{(I)})-\Theta(-\bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_l^{(I)})\right)\Big)\\ =&-\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\left(\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_k^{(I)}+\bar{\varepsilon}_l^{(I)}\right)^{-1}\mathrm{e}^{-|\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_k^{(I)}||\tau_1-\tau_2|}\,(\phi_m^{(\mathrm{P})}(x_1))^*\,\phi_m^{(\mathrm{P})}(x_2)\\ &\qquad\Theta(\bar{\varepsilon}_{k+m}^{(I)})\Theta(-\bar{\varepsilon}_k^{(I)})\left(\Theta(\bar{\varepsilon}_{l+m}^{(I)})-\Theta(\bar{\varepsilon}_l^{(I)})\right), \qquad\text{(B.15)}\end{aligned}$$

where we shifted the k and l sums for the term depending on $\Theta_\tau(\tau_2-\tau_1)$ in the last step. For odd particle numbers or $I=\mathrm{P}$ the shift is $k\to -k-m$ and $l\to -l-m$ and for even particle numbers or $I=\mathrm{A}$ the shift is $k\to -k-m-1$ and $l\to -l-m-1$. Moreover, we used Eqs. (B.12) again to remove the $\Theta_\tau(\tau)$'s. We also used relation (B.9) to simplify

$$\Theta(\bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_l^{(I)})-\Theta(-\bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_l^{(I)})=\Theta(\bar{\varepsilon}_{l+m}^{(I)})-\Theta(\bar{\varepsilon}_l^{(I)}). \tag{B.16}$$

Going on with the second line (B.14) we find:

$$\begin{aligned}&\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\left(\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_k^{(I)}+\bar{\varepsilon}_l^{(I)}\right)^{-1}\mathrm{e}^{-|\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_l^{(I)}||\tau_1-\tau_2|}\,(\phi_m^{(\mathrm{P})}(x_1))^*\,\phi_m^{(\mathrm{P})}(x_2)\\ &\qquad\Big(\ \Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}_{l+m}^{(I)}+\bar{\varepsilon}_k^{(I)}-\bar{\varepsilon}_l^{(I)})\Theta(-\bar{\varepsilon}_k^{(I)})\left(\Theta(\bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_l^{(I)})-\Theta(-\bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_l^{(I)})\right)\\ &\qquad+\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_k^{(I)}+\epsilon_l)\Theta(\bar{\varepsilon}_k^{(I)})\left(\Theta(\bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_l^{(I)})-\Theta(-\bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_l^{(I)})\right)\Big)\\ =&\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\left(\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_k^{(I)}+\bar{\varepsilon}_l^{(I)}\right)^{-1}\mathrm{e}^{-|\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_l^{(I)}||\tau_1-\tau_2|}\,(\phi_m^{(\mathrm{P})}(x_1))^*\,\phi_m^{(\mathrm{P})}(x_2)\\ &\qquad\Big(\ \Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}_{l+m}^{(I)}+\bar{\varepsilon}_k^{(I)}-\bar{\varepsilon}_l^{(I)})\Theta(-\bar{\varepsilon}_k^{(I)})\Theta(\bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_l^{(I)})\\ &\qquad-\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_k^{(I)}+\epsilon_l)\Theta(\bar{\varepsilon}_k^{(I)})\Theta(-\bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_l^{(I)})\Big). \qquad\text{(B.17)}\end{aligned}$$

Here we used again Eqs. (B.5) to simplify the $\Theta(\varepsilon)$-functions.

We now combine line (B.17) and line (B.7) and obtain a result that is not depending on a $\Theta_\tau(\tau)$ function:

$$
\begin{aligned}
&\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\left(\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l}\right)^{-1}\ \mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{l}||\tau_1-\tau_2|}\ (\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\Big\{\ \Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_{l+m}+\bar{\varepsilon}^{(I)}_{k}-\bar{\varepsilon}^{(I)}_{l})\Theta(-\bar{\varepsilon}^{(I)}_{k})\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l})\\
&\qquad\ -\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\epsilon_l)\Theta(\bar{\varepsilon}^{(I)}_{k})\Theta(-\bar{\varepsilon}^{(I)}_{l+m})\Theta(\bar{\varepsilon}^{(I)}_{l})\Big)\\
&\qquad\ -\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l})\ \left(\Theta(\bar{\varepsilon}^{(I)}_{l+m}+\bar{\varepsilon}^{(I)}_{k}-\bar{\varepsilon}^{(I)}_{l})-\Theta(\bar{\varepsilon}^{(I)}_{k+m})\right)\\
&\qquad\ -\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{l+m})\Theta(\bar{\varepsilon}^{(I)}_{l})\ \left(\Theta(-\bar{\varepsilon}^{(I)}_{k+m})-\Theta(-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l})\right)\Big\}\\
=&\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\left(\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l}\right)^{-1}\ \mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{l}||\tau_1-\tau_2|}\ (\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\Big\{-\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l})\ \left(\left((1-\Theta(-\bar{\varepsilon}^{(I)}_{k})\right)\Theta(\bar{\varepsilon}^{(I)}_{l+m}+\bar{\varepsilon}^{(I)}_{k}-\bar{\varepsilon}^{(I)}_{l})-\Theta(\bar{\varepsilon}^{(I)}_{k+m})\right)\\
&\qquad\ -\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{l+m})\Theta(\bar{\varepsilon}^{(I)}_{l})\ \left(\Theta(-\bar{\varepsilon}^{(I)}_{k+m})-\left((1-\Theta(\bar{\varepsilon}^{(I)}_{k})\right)\Theta(-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l})\right)\Big\}\\
=&\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\left(\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l}\right)^{-1}\ \mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{l}||\tau_1-\tau_2|}\ (\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\Big\{-\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l})\ \left(\Theta(\bar{\varepsilon}^{(I)}_{k})-\Theta(\bar{\varepsilon}^{(I)}_{k+m})\right)\\
&\qquad\ -\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{l+m})\Theta(\bar{\varepsilon}^{(I)}_{l})\ \left(\Theta(-\bar{\varepsilon}^{(I)}_{k+m})-\Theta(-\bar{\varepsilon}^{(I)}_{k})\right)\Big\}\\
=&-\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\left(\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l}\right)^{-1}\ \mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{l}||\tau_1-\tau_2|}\ (\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l})\ \left(\Theta(\bar{\varepsilon}^{(I)}_{k})-\Theta(\bar{\varepsilon}^{(I)}_{k+m})\right).
\end{aligned}
\tag{B.18}
$$

In the second to last step we used Eq. (B.5) to simplify the $\Theta(\varepsilon)$-functions and in the last step we shifted the k and l sums for the term depending on $\Theta_\tau(\tau_2-\tau_1)$. For odd particle numbers or $I=\mathrm{P}$ the shift is $k\to -k-m$ and $l\to -l-m$ and for even particle numbers or $I=\mathrm{A}$ the shift is $k\to -k-m-1$ and $l\to -l-m-1$. We then used Eqs. (B.12) to remove the $\Theta_\tau(\tau)$'s.

To obtain the final result for $\mathscr{G}^{(2,1)}$, we combine Eqs. (B.11), (B.15) and (B.18):

$$
\begin{aligned}
&\mathscr{G}^{(2,1)}(\tau_1,x_1,\tau_2,x_2)\\
&\quad=\ \frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k}\ \mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_{k}||\tau_1-\tau_2|}\,|\tau_1-\tau_2|\ \Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_{k})\ (\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\quad\ -\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\left(\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l}\right)^{-1}\ \mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_{k}||\tau_1-\tau_2|}\ (\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_{k})\ \left(\Theta(\bar{\varepsilon}^{(I)}_{l+m})-\Theta(\bar{\varepsilon}^{(I)}_{l})\right)\\
&\quad\ -\frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\left(\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{k}+\bar{\varepsilon}^{(I)}_{l}\right)^{-1}\ \mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{l+m}-\bar{\varepsilon}^{(I)}_{l}||\tau_1-\tau_2|}\ (\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\Theta(\bar{\varepsilon}^{(I)}_{l+m})\Theta(-\bar{\varepsilon}^{(I)}_{l})\ \left(\Theta(\bar{\varepsilon}^{(I)}_{k})-\Theta(\bar{\varepsilon}^{(I)}_{k+m})\right)\\
&\quad=\ \frac{1}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k}\ \mathrm{e}^{-|\varepsilon^{(I)}_{k+m}-\varepsilon^{(I)}_{k}||\tau_1-\tau_2|}\,|\tau_1-\tau_2|\ \Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_{k})\ (\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\quad\ -\frac{2}{L^2}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k\neq l}\left(\varepsilon^{(I)}_{k+m}-\varepsilon^{(I)}_{l+m}-\varepsilon^{(I)}_{k}+\varepsilon^{(I)}_{l}\right)^{-1}\ \mathrm{e}^{-|\varepsilon^{(I)}_{k+m}-\varepsilon^{(I)}_{k}||\tau_1-\tau_2|}\ (\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_{k})\ \left(\Theta(\bar{\varepsilon}^{(I)}_{l+m})-\Theta(\bar{\varepsilon}^{(I)}_{l})\right).
\end{aligned}
\tag{B.19}
$$

In the second to last step we interchanged the summation indices k and l in the third line which is just a relabeling of the variables and does not change the result. By this transformation it becomes clear that the second and the third line are identical. In addition, we also used the relation $\bar{\varepsilon}_k^{(I)} - \bar{\varepsilon}_l^{(I)} = \varepsilon_k^{(I)} - \varepsilon_l^{(I)}$.

The final result for $\mathscr{G}^{(2,1)}$ is given by

$$\begin{aligned}
&\mathscr{G}^{(2,1)}(\tau_1, x_1, 0, x_2) \\
&\quad = -\frac{1}{L^2} \sum_{m\neq 0} \mathfrak{U}_{m,m} (\phi_m^{(P)}(x_1))^* \phi_m^{(P)}(x_2) \Bigg\{ \Bigg(\sum_k \theta(-\bar{\varepsilon}_k^{(I)}) \theta(\bar{\varepsilon}_{k+m}^{(I)}) |\tau_1| \mathrm{e}^{-|\varepsilon_{k+m}^{(I)} - \varepsilon_k^{(I)}||\tau_1|} \\
&\qquad - 2 \sum_{k\neq l} \frac{1}{\varepsilon_{k+m}^{(I)} - \varepsilon_{l+m}^{(I)} + \varepsilon_l^{(I)} - \varepsilon_k^{(I)}} \theta(\bar{\varepsilon}_{k+m}^{(I)}) \theta(-\bar{\varepsilon}_k^{(I)}) \Big(\theta(-\varepsilon_l^{(I)}) - \theta(-\varepsilon_{l+m}^{(I)}) \Big) \mathrm{e}^{-|\varepsilon_{k+m}^{(I)} - \varepsilon_k^{(I)}||\tau_1|} \Bigg\},
\end{aligned} \tag{B.20}$$

where we set $\tau_2 = 0$ for convenience.

For the calculation of the second-order correction to the ground-state density we need the result for $\mathscr{G}^{(2,1)}$ for $\tau_1 = \tau_2 = 0$:

$$\begin{aligned}
&\mathscr{G}^{(2,1)}(0, x_1, 0, x_2) \\
&\quad = \frac{2}{L^2} \sum_{m\neq 0} \mathfrak{U}_{m,m} (\phi_m^{(P)}(x_1))^* \phi_m^{(P)}(x_2) \sum_{k\neq l} \frac{1}{\varepsilon_{k+m}^{(I)} - \varepsilon_{l+m}^{(I)} + \varepsilon_l^{(I)} - \varepsilon_k^{(I)}} \theta(\bar{\varepsilon}_{k+m}^{(I)}) \theta(-\bar{\varepsilon}_k^{(I)}) \Big(\theta(-\varepsilon_l^{(I)}) - \theta(-\varepsilon_{l+m}^{(I)}) \Big).
\end{aligned} \tag{B.21}$$

In our numerical calculations in Sec. 6.4 we use the a-th Fourier coefficient of $\mathscr{G}^{(2,1)}$ given by

$$\begin{aligned}
\tilde{\mathscr{G}}_{a,a}^{(2,1)}(\omega) = &\frac{2}{L^2} \mathfrak{U}_{a,a} \Bigg\{ \sum_k \theta(-\bar{\varepsilon}_k^{(I)}) \theta(\bar{\varepsilon}_{k+a}^{(I)}) \frac{|\varepsilon_{k+a}^{(I)} - \varepsilon_k^{(I)}|^2 - \omega^2}{(\omega^2 + |\varepsilon_{k+a}^{(I)} - \varepsilon_k^{(I)}|^2)^2} \\
&- 2 \sum_{k\neq l} \frac{1}{\varepsilon_{k+a}^{(I)} - \varepsilon_{l+a}^{(I)} + \varepsilon_l^{(I)} - \varepsilon_k^{(I)}} \theta(\bar{\varepsilon}_{k+a}^{(I)}) \theta(-\bar{\varepsilon}_k^{(I)}) \Big(\theta(-\varepsilon_l^{(I)}) - \theta(-\varepsilon_{l+a}^{(I)}) \Big) \frac{|\varepsilon_{k+a}^{(I)} - \varepsilon_k^{(I)}|}{\omega^2 + |\varepsilon_{k+a}^{(I)} - \varepsilon_k^{(I)}|^2} \Bigg\}.
\end{aligned} \tag{B.22}$$

Let us now come to the second term we need in order to calculate the first order perturbative correction of the density-density correlation function, namely $\mathscr{G}^{(4,1)}$:

$$\begin{aligned}
&\mathscr{G}^{(4,1)}(\tau_1, x_1, \tau_2, x_2) \\
&\quad = \frac{1}{2} \int_{\tau_3} \int_{x_3} \int_{x_4} \mathfrak{U}(x_3 - x_4)\, G^{(4,0)}(\tau_3, x_4, \tau_3, x_3, \tau_1, x_1, \tau_2, x_2) \\
&\quad = \frac{1}{2} \int_{\tau_3} \int_{x_3} \int_{x_4} \sum_m \mathfrak{U}_{m,m} (\phi_m^{(\mathrm{P})}(x_3))^* \phi_m^{(\mathrm{P})}(x_4)\, G^{(4,0)}(\tau_3, x_4, \tau_3, x_3, \tau_1, x_1, \tau_2, x_2) \\
&\quad = -\frac{1}{2} \int_{\tau_3} \int_{x_3} \int_{x_4} \sum_m \mathfrak{U}_{m,m} (\phi_m^{(\mathrm{P})}(x_3))^* \phi_m^{(\mathrm{P})}(x_4) \\
&\qquad \Big\{ \Delta_{\lambda=0}^{(I)}(\tau_3, x_4, \tau_3, x_3)\, \Delta_{\lambda=0}^{(I)}(\tau_3, x_3, \tau_1, x_1)\, \Delta_{\lambda=0}^{(I)}(\tau_1, x_1, \tau_2, x_2)\, \Delta_{\lambda=0}^{(I)}(\tau_2, x_2, \tau_3, x_4) && \text{(B.23)} \\
&\qquad + \Delta_{\lambda=0}^{(I)}(\tau_3, x_3, \tau_3, x_4)\, \Delta_{\lambda=0}^{(I)}(\tau_3, x_4, \tau_1, x_1)\, \Delta_{\lambda=0}^{(I)}(\tau_1, x_1, \tau_2, x_2)\, \Delta_{\lambda=0}^{(I)}(\tau_2, x_2, \tau_3, x_3) && \text{(B.24)} \\
&\qquad + \Delta_{\lambda=0}^{(I)}(\tau_3, x_4, \tau_3, x_3)\, \Delta_{\lambda=0}^{(I)}(\tau_3, x_3, \tau_2, x_2)\, \Delta_{\lambda=0}^{(I)}(\tau_2, x_2, \tau_1, x_1)\, \Delta_{\lambda=0}^{(I)}(\tau_1, x_1, \tau_3, x_4) && \text{(B.25)} \\
&\qquad + \Delta_{\lambda=0}^{(I)}(\tau_3, x_3, \tau_3, x_4)\, \Delta_{\lambda=0}^{(I)}(\tau_3, x_4, \tau_2, x_2)\, \Delta_{\lambda=0}^{(I)}(\tau_2, x_2, \tau_1, x_1)\, \Delta_{\lambda=0}^{(I)}(\tau_1, x_1, \tau_3, x_3) && \text{(B.26)} \\
&\qquad + \Delta_{\lambda=0}^{(I)}(\tau_3, x_4, \tau_1, x_1)\, \Delta_{\lambda=0}^{(I)}(\tau_1, x_1, \tau_3, x_3)\, \Delta_{\lambda=0}^{(I)}(\tau_3, x_3, \tau_2, x_2)\, \Delta_{\lambda=0}^{(I)}(\tau_2, x_2, \tau_3, x_4) && \text{(B.27)} \\
&\qquad + \Delta_{\lambda=0}^{(I)}(\tau_3, x_3, \tau_1, x_1)\, \Delta_{\lambda=0}^{(I)}(\tau_1, x_1, \tau_3, x_4)\, \Delta_{\lambda=0}^{(I)}(\tau_3, x_4, \tau_2, x_2)\, \Delta_{\lambda=0}^{(I)}(\tau_2, x_2, \tau_3, x_3) \Big\}, && \text{(B.28)}
\end{aligned}$$

where we first used Eqs. (5.5) and (5.6) and then plugged in $G_{\lambda=0}^{(4)}$ given in Eq. (3.32).

To simplify this equation we can now exchange x_3 and x_4 in lines (B.24), (B.26) and (B.28). This does not change the result because it is just a relabelling of the integral variables. We will then shift the sum in these lines so that $m \to -m$ and use that $\mathfrak{U}_{m,m} \equiv \mathfrak{U}_{-m,-m}$ and $\phi_m^{(\mathrm{P})}(x) \equiv (\phi_{-m}^{(\mathrm{P})}(x))^*$. After these transformations we can see that line (B.24) is now equal to line (B.23), line (B.26) to line (B.25) and line (B.28) to line (B.27). With this, we can simplify $\mathcal{G}^{(4,1)}(\tau_1, x_1, \tau_2, x_2)$ to:

$$
\begin{aligned}
&\mathcal{G}^{(4,1)}(\tau_1, x_1, \tau_2, x_2) \\
&\quad = -\int_{\tau_3}\int_{x_3}\int_{x_4} \sum_m \mathfrak{U}_{m,m} (\phi_m^{(\mathrm{P})}(x_3))^* \phi_m^{(\mathrm{P})}(x_4) \\
&\qquad \Big\{ \Delta^{(I)}_{\lambda=0}(\tau_3, x_4, \tau_3, x_3)\, \Delta^{(I)}_{\lambda=0}(\tau_3, x_3, \tau_1, x_1)\, \Delta^{(I)}_{\lambda=0}(\tau_1, x_1, \tau_2, x_2)\, \Delta^{(I)}_{\lambda=0}(\tau_2, x_2, \tau_3, x_4) && \text{(B.29)} \\
&\qquad + \Delta^{(I)}_{\lambda=0}(\tau_3, x_4, \tau_3, x_3)\, \Delta^{(I)}_{\lambda=0}(\tau_3, x_3, \tau_2, x_2)\, \Delta^{(I)}_{\lambda=0}(\tau_2, x_2, \tau_1, x_1)\, \Delta^{(I)}_{\lambda=0}(\tau_1, x_1, \tau_3, x_4) && \text{(B.30)} \\
&\qquad + \Delta^{(I)}_{\lambda=0}(\tau_3, x_4, \tau_1, x_1)\, \Delta^{(I)}_{\lambda=0}(\tau_1, x_1, \tau_3, x_3)\, \Delta^{(I)}_{\lambda=0}(\tau_3, x_3, \tau_2, x_2)\, \Delta^{(I)}_{\lambda=0}(\tau_2, x_2, \tau_3, x_4) \Big\}. && \text{(B.31)}
\end{aligned}
$$

We begin with the evaluation of (B.29):

$$
\begin{aligned}
&-\int_{\tau_3}\int_{x_3}\int_{x_4} \sum_m \mathfrak{U}_{m,m} (\phi_m^{(\mathrm{P})}(x_3))^* \phi_m^{(\mathrm{P})}(x_4) \\
&\qquad \Delta^{(I)}_{\lambda=0}(\tau_3, x_4, \tau_3, x_3)\, \Delta^{(I)}_{\lambda=0}(\tau_3, x_3, \tau_1, x_1)\, \Delta^{(I)}_{\lambda=0}(\tau_1, x_1, \tau_2, x_2)\, \Delta^{(I)}_{\lambda=0}(\tau_2, x_2, \tau_3, x_4) \\
&= -\int_{\tau_3}\int_{x_3}\int_{x_4} \sum_m \mathfrak{U}_{m,m} (\phi_m^{(\mathrm{P})}(x_3))^* \phi_m^{(\mathrm{P})}(x_4) \sum_{k_1 \dots k_4} \int_{\omega_1} \cdots \int_{\omega_4} \left(-\mathrm{i}\,\omega_1 + \bar{\varepsilon}^{(I)}_{k_1}\right)^{-1} \left(-\mathrm{i}\,\omega_2 + \bar{\varepsilon}^{(I)}_{k_2}\right)^{-1} \\
&\qquad \left(-\mathrm{i}\,\omega_3 + \bar{\varepsilon}^{(I)}_{k_3}\right)^{-1} \left(-\mathrm{i}\,\omega_4 + \bar{\varepsilon}^{(I)}_{k_4}\right)^{-1} \mathrm{e}^{-\mathrm{i}\,\omega_1(\tau_3-\tau_3)} \mathrm{e}^{-\mathrm{i}\,\omega_2(\tau_3-\tau_1)} \mathrm{e}^{-\mathrm{i}\,\omega_3(\tau_1-\tau_2)} \mathrm{e}^{-\mathrm{i}\,\omega_4(\tau_2-\tau_3)} \\
&\qquad (\phi^{(I)}_{k_1}(x_4))^* \phi^{(I)}_{k_1}(x_3) (\phi^{(I)}_{k_2}(x_3))^* \phi^{(I)}_{k_2}(x_1) (\phi^{(I)}_{k_3}(x_1))^* \phi^{(I)}_{k_3}(x_2) (\phi^{(I)}_{k_4}(x_2))^* \phi^{(I)}_{k_4}(x_4) \\
&= -\sum_m \mathfrak{U}_{m,m} \sum_{k_1 \dots k_4} \int_{\omega_1} \cdots \int_{\omega_4} \left(-\mathrm{i}\,\omega_1 + \bar{\varepsilon}^{(I)}_{k_1}\right)^{-1} \left(-\mathrm{i}\,\omega_2 + \bar{\varepsilon}^{(I)}_{k_2}\right)^{-1} \left(-\mathrm{i}\,\omega_3 + \bar{\varepsilon}^{(I)}_{k_3}\right)^{-1} \left(-\mathrm{i}\,\omega_4 + \bar{\varepsilon}^{(I)}_{k_4}\right)^{-1} \\
&\qquad \frac{\delta_{m+k_1,k_4}}{\sqrt{L}} \frac{\delta_{m+k_1,k_2}}{\sqrt{L}}\, 2\pi\,\delta(\omega_2-\omega_4)\, \mathrm{e}^{\mathrm{i}\omega_2\tau_1} \mathrm{e}^{-\mathrm{i}\,\omega_3(\tau_1-\tau_2)} \mathrm{e}^{-\mathrm{i}\,\omega_4\tau_2}\, \phi^{(\mathrm{P})}_{k_2}(x_1) (\phi^{(\mathrm{P})}_{k_3}(x_1))^* \phi^{(\mathrm{P})}_{k_3}(x_2) (\phi^{(\mathrm{P})}_{k_4}(x_2))^* \\
&= -\frac{1}{L}\sum_m \mathfrak{U}_{m,m} \sum_{k,l} \int_{\omega_1} \cdots \int_{\omega_3} \left(-\mathrm{i}\,\omega_1 + \bar{\varepsilon}^{(I)}_{k}\right)^{-1} \left(-\mathrm{i}\,\omega_2 + \bar{\varepsilon}^{(I)}_{k+m}\right)^{-1} \left(-\mathrm{i}\,\omega_3 + \bar{\varepsilon}^{(I)}_{l}\right)^{-1} \left(-\mathrm{i}\,\omega_2 + \bar{\varepsilon}^{(I)}_{k+m}\right)^{-1} \\
&\qquad \mathrm{e}^{-\mathrm{i}\,\omega_2(\tau_2-\tau_1)} \mathrm{e}^{-\mathrm{i}\,\omega_3(\tau_1-\tau_2)}\, (\phi^{(\mathrm{P})}_{k+m}(x_2))^* \phi^{(\mathrm{P})}_{k+m}(x_1) (\phi^{(\mathrm{P})}_{l}(x_1))^* \phi^{(\mathrm{P})}_{l}(x_2) \\
&= \frac{1}{L}\sum_m \mathfrak{U}_{m,m} \sum_{k,l} \Theta(-\bar{\varepsilon}^{(I)}_k)\, \mathrm{e}^{\bar{\varepsilon}^{(I)}_{k+m}(\tau_1-\tau_2)} |\tau_1-\tau_2| \left(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar{\varepsilon}^{(I)}_{k+m}) + \Theta_\tau(\tau_2-\tau_1)\Theta(\bar{\varepsilon}^{(I)}_{k+m})\right) \\
&\qquad \mathrm{e}^{-\bar{\varepsilon}^{(I)}_l(\tau_1-\tau_2)} \left(\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_l) - \Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_l)\right) (\phi^{(\mathrm{P})}_{k+m}(x_2))^* \phi^{(\mathrm{P})}_{k+m}(x_1) (\phi^{(\mathrm{P})}_{l}(x_1))^* \phi^{(\mathrm{P})}_{l}(x_2) \\
&= \frac{1}{L}\sum_m \mathfrak{U}_{m,m} \sum_{k,l} \Theta(-\bar{\varepsilon}^{(I)}_k)\, \mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{k+m} - \bar{\varepsilon}^{(I)}_l||\tau_1-\tau_2|} |\tau_1-\tau_2|\, (\phi^{(\mathrm{P})}_{k+m}(x_2))^* \phi^{(\mathrm{P})}_{k+m}(x_1) (\phi^{(\mathrm{P})}_{l}(x_1))^* \phi^{(\mathrm{P})}_{l}(x_2) \\
&\qquad \left(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar{\varepsilon}^{(I)}_{k+m})\Theta(\bar{\varepsilon}^{(I)}_l) + \Theta_\tau(\tau_2-\tau_1)\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_l)\right). && \text{(B.32)}
\end{aligned}
$$

In the ω_1 integral the factor $\mathrm{e}^{-\mathrm{i}\,\omega_1(\tau_3-\tau_3)}$ is equal to one. To solve the ω_1 integral we need to have a look at the limits $\tau_3 - \tau_3 = \delta_- < 0$ and $\tau_3 - \tau_3 = \delta_+ > 0$:

$$
\lim_{\delta_- \to 0^-} \int_{\omega_1} \left(-\mathrm{i}\,\omega_1 + \bar{\varepsilon}^{(I)}_k\right)^{-1} \mathrm{e}^{-\omega_1\delta_-} = -\Theta(-\bar{\varepsilon}^{(I)}_k) \qquad \text{(B.33)}
$$

$$
\lim_{\delta_+ \to 0^+} \int_{\omega_1} \left(-\mathrm{i}\,\omega_1 + \bar{\varepsilon}^{(I)}_k\right)^{-1} \mathrm{e}^{-\omega_1\delta_+} = \Theta(\bar{\varepsilon}^{(I)}_k) = 1 - \Theta(-\bar{\varepsilon}^{(I)}_k). \qquad \text{(B.34)}
$$

As we can observe immediately, the limit in both cases is not the same. However, it is possible to show that the term (B.32) vanishes if we plug it in the one from (B.34). The remaining term is the one with $-\Theta(-\bar{\varepsilon}_k^{(I)})$ which is identical with the result (B.33).

Let us now come to line (B.30). The only difference between this line and line (B.29) is that τ_1 and τ_2 and x_1 and x_2 are reversed. So it is possible to take the result (B.32) and just exchange τ_1 and τ_2 as well as x_1 and x_2 :

$$
\begin{aligned}
&-\int_{\tau_3}\int_{x_3}\int_{x_4}\sum_m \mathfrak{U}_{m,m}(\phi_m^{(\mathrm{P})}(x_3))^*\phi_m^{(\mathrm{P})}(x_4)\\
&\qquad\qquad \Delta^{(I)}_{\lambda=0}(\tau_3,x_4,\tau_3,x_3)\,\Delta^{(I)}_{\lambda=0}(\tau_3,x_3,\tau_2,x_2)\,\Delta^{(I)}_{\lambda=0}(\tau_2,x_2,\tau_1,x_1)\,\Delta^{(I)}_{\lambda=0}(\tau_1,x_1,\tau_3,x_4)\\
&=\frac{1}{L}\sum_m \mathfrak{U}_{m,m}\sum_{k,l}\Theta(-\bar{\varepsilon}_k^{(I)})\,\mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_l||\tau_1-\tau_2|}|\tau_1-\tau_2|\,(\phi^{(\mathrm{P})}_{k+m}(x_1))^*\phi^{(\mathrm{P})}_{k+m}(x_2)(\phi^{(\mathrm{P})}_l(x_2))^*\phi^{(\mathrm{P})}_l(x_1)\\
&\qquad\Big(\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{k+m})\Theta(\bar{\varepsilon}^{(I)}_l)+\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_l)\Big)\\
&=\frac{1}{L}\sum_m \mathfrak{U}_{m,m}\sum_{k,l}\Theta(-\bar{\varepsilon}_k^{(I)})\,\mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_l||\tau_1-\tau_2|}|\tau_1-\tau_2|\,(\phi^{(\mathrm{P})}_{k+m}(x_2))^*\phi^{(\mathrm{P})}_{k+m}(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\\
&\qquad\Big(\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{k+m})\Theta(\bar{\varepsilon}^{(I)}_l)+\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_l)\Big)\,.
\end{aligned}
\tag{B.35}
$$

In the last step we have used the fact that we can shift the m-sum so that $m\to -m$ and use that $\mathfrak{U}_{m,m}\equiv\mathfrak{U}_{-m,-m}$. For odd particle numbers we shift the k- and l-sum so that $k\to -k$ and $l\to -l$ and for even particle numbers we shift the k- and l-sum so that $k\to -k-1$ and $l\to -l-1$. We then used that $\phi^{(\mathrm{P})}_k(x)\equiv(\phi^{(\mathrm{P})}_{-k}(x))^*$, $(\phi^{(\mathrm{P})}_{k-1}(x_1))^*\phi^{(\mathrm{P})}_{k-1}(x_2)\equiv(\phi^{(\mathrm{P})}_k(x_1))^*\phi^{(\mathrm{P})}_k(x_2)$ and Eq. (B.12). Now it is easy to see that the terms (B.32) and (B.35) are only different in the timelike Θ-functions and that it is now possible to write the result independent of these functions:

$$
\begin{aligned}
&-\int_{\tau_3}\int_{x_3}\int_{x_4}\sum_m \mathfrak{U}_{m,m}(\phi_m^{(\mathrm{P})}(x_3))^*\phi_m^{(\mathrm{P})}(x_4)\\
&\qquad\Big\{\;\Delta^{(I)}_{\lambda=0}(\tau_3,x_4,\tau_3,x_3)\,\Delta^{(I)}_{\lambda=0}(\tau_3,x_3,\tau_1,x_1)\,\Delta^{(I)}_{\lambda=0}(\tau_1,x_1,\tau_2,x_2)\,\Delta^{(I)}_{\lambda=0}(\tau_2,x_2,\tau_3,x_4)\\
&\qquad+\Delta^{(I)}_{\lambda=0}(\tau_3,x_4,\tau_3,x_3)\,\Delta^{(I)}_{\lambda=0}(\tau_3,x_3,\tau_2,x_2)\,\Delta^{(I)}_{\lambda=0}(\tau_2,x_2,\tau_1,x_1)\,\Delta^{(I)}_{\lambda=0}(\tau_1,x_1,\tau_3,x_4)\Big\}\\
&=\frac{1}{L}\sum_m \mathfrak{U}_{m,m}\sum_{k,l}\Theta(-\bar{\varepsilon}_k^{(I)})\,\mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_l||\tau_1-\tau_2|}|\tau_1-\tau_2|\,(\phi^{(\mathrm{P})}_{k+m}(x_2))^*\phi^{(\mathrm{P})}_{k+m}(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\\
&\qquad\Big\{\;\Big(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar{\varepsilon}^{(I)}_{k+m})\Theta(\bar{\varepsilon}^{(I)}_l)+\Theta_\tau(\tau_2-\tau_1)\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_l)\Big)\\
&\qquad+\Big(\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar{\varepsilon}^{(I)}_{k+m})\Theta(\bar{\varepsilon}^{(I)}_l)+\Theta_\tau(\tau_1-\tau_2)\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_l)\Big)\Big\}\\
&=\frac{1}{L}\sum_m \mathfrak{U}_{m,m}\sum_{k,l}\mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_l||\tau_1-\tau_2|}|\tau_1-\tau_2|\,(\phi^{(\mathrm{P})}_{k+m}(x_2))^*\phi^{(\mathrm{P})}_{k+m}(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\\
&\qquad\Big(\Theta(-\bar{\varepsilon}^{(I)}_{k+m})\Theta(\bar{\varepsilon}^{(I)}_l)+\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_l)\Big)\;\Theta(-\bar{\varepsilon}^{(I)}_k)\\
&=\quad\frac{1}{L}\mathfrak{U}_{0,0}\sum_{k,l}\mathrm{e}^{-|\bar{\varepsilon}^{(I)}_k-\bar{\varepsilon}^{(I)}_l||\tau_1-\tau_2|}|\tau_1-\tau_2|\,(\phi^{(\mathrm{P})}_k(x_2))^*\phi^{(\mathrm{P})}_k(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\,\Theta(-\bar{\varepsilon}^{(I)}_k)\Theta(\bar{\varepsilon}^{(I)}_l)\\
&\quad+\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\mathrm{e}^{-|\bar{\varepsilon}^{(I)}_{k+m}-\bar{\varepsilon}^{(I)}_l||\tau_1-\tau_2|}|\tau_1-\tau_2|\,(\phi^{(\mathrm{P})}_{k+m}(x_2))^*\phi^{(\mathrm{P})}_{k+m}(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\\
&\qquad\Big(\Theta(-\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_k)\Theta(\bar{\varepsilon}^{(I)}_l)+\Theta(\bar{\varepsilon}^{(I)}_{k+m})\Theta(-\bar{\varepsilon}^{(I)}_k)\Theta(-\bar{\varepsilon}^{(I)}_l)\Big)\,.
\end{aligned}
\tag{B.36}
$$

Note that we just split up the result into one term with $m=0$ and the terms $m\neq 0$ in the last step.

Now we come to the evaluation of the last remaining term to calculate for $\mathcal{G}^{(4,1)}(\tau_1,x_1,\tau_2,x_2)$ given in line (B.31):

$$
\begin{aligned}
&-\int_{\tau_3}\int_{x_3}\int_{x_4}\sum_m \mathfrak{U}_{m,m}\,(\phi_m^{(\mathrm{P})}(x_3))^*\phi_m^{(\mathrm{P})}(x_4)\\
&\qquad\qquad \Delta^{(I)}_{\lambda=0}(\tau_3,x_4,\tau_1,x_1)\,\Delta^{(I)}_{\lambda=0}(\tau_1,x_1,\tau_3,x_3)\,\Delta^{(I)}_{\lambda=0}(\tau_3,x_3,\tau_2,x_2)\,\Delta^{(I)}_{\lambda=0}(\tau_2,x_2,\tau_3,x_4)\\
&=-\int_{\tau_3}\int_{x_3}\int_{x_4}\sum_m \mathfrak{U}_{m,m}\,(\phi_m^{(\mathrm{P})}(x_3))^*\phi_m^{(\mathrm{P})}(x_4)\sum_{k_1\dots k_4}\int_{\omega_1}\cdots\int_{\omega_4}\left(-\mathrm{i}\,\omega_1+\bar\varepsilon^{(I)}_{k_1}\right)^{-1}\left(-\mathrm{i}\,\omega_2+\bar\varepsilon^{(I)}_{k_2}\right)^{-1}\\
&\qquad\left(-\mathrm{i}\,\omega_3+\bar\varepsilon^{(I)}_{k_3}\right)^{-1}\left(-\mathrm{i}\,\omega_4+\bar\varepsilon^{(I)}_{k_4}\right)^{-1}\;\mathrm{e}^{-\mathrm{i}\,\omega_1(\tau_3-\tau_1)}\,\mathrm{e}^{-\mathrm{i}\,\omega_2(\tau_1-\tau_3)}\,\mathrm{e}^{-\mathrm{i}\,\omega_3(\tau_3-\tau_2)}\,\mathrm{e}^{-\mathrm{i}\,\omega_4(\tau_2-\tau_3)}\\
&\qquad(\phi^{(I)}_{k_1}(x_4))^*\phi^{(I)}_{k_1}(x_1)(\phi^{(I)}_{k_2}(x_1))^*\phi^{(I)}_{k_2}(x_3)(\phi^{(I)}_{k_3}(x_3))^*\phi^{(I)}_{k_3}(x_2)(\phi^{(I)}_{k_4}(x_2))^*\phi^{(I)}_{k_4}(x_4)\\
&=-\sum_m \mathfrak{U}_{m,m}\sum_{k_1\dots k_4}\int_{\omega_1}\cdots\int_{\omega_4}\left(-\mathrm{i}\,\omega_1+\bar\varepsilon^{(I)}_{k_1}\right)^{-1}\left(-\mathrm{i}\,\omega_2+\bar\varepsilon^{(I)}_{k_2}\right)^{-1}\left(-\mathrm{i}\,\omega_3+\bar\varepsilon^{(I)}_{k_3}\right)^{-1}\left(-\mathrm{i}\,\omega_4+\bar\varepsilon^{(I)}_{k_4}\right)^{-1}\\
&\qquad\frac{\delta_{k_1+m,k_4}}{\sqrt{L}}\,\frac{\delta_{k_2+m,k_3}}{\sqrt{L}}\,2\pi\,\delta(\omega_1-\omega_2+\omega_3-\omega_4)\\
&\qquad\mathrm{e}^{\mathrm{i}\,\omega_1\tau_1}\,\mathrm{e}^{-\mathrm{i}\,\omega_2\tau_1}\,\mathrm{e}^{\mathrm{i}\,\omega_3\tau_2}\,\mathrm{e}^{-\mathrm{i}\,\omega_4\tau_2}\;\phi^{(\mathrm{P})}_{k_1}(x_1)(\phi^{(\mathrm{P})}_{k_2}(x_1))^*\,\phi^{(\mathrm{P})}_{k_3}(x_2)(\phi^{(\mathrm{P})}_{k_4}(x_2))^*\\
&=-\frac{1}{L}\sum_m \mathfrak{U}_{m,m}\sum_{k,l}\int_{\omega_1}\cdots\int_{\omega_3}\left(-\mathrm{i}\,\omega_1+\bar\varepsilon^{(I)}_{k}\right)^{-1}\left(-\mathrm{i}\,\omega_2+\bar\varepsilon^{(I)}_{l}\right)^{-1}\left(-\mathrm{i}\,\omega_3+\bar\varepsilon^{(I)}_{l+m}\right)^{-1}\left(-\mathrm{i}\,(\omega_1-\omega_2+\omega_3)+\bar\varepsilon^{(I)}_{k+m}\right)^{-1}\\
&\qquad\mathrm{e}^{\mathrm{i}\,\omega_1\tau_1}\mathrm{e}^{-\mathrm{i}\,\omega_2\tau_1}\mathrm{e}^{\mathrm{i}\,\omega_3\tau_2}\mathrm{e}^{-\mathrm{i}\,(\omega_1-\omega_2+\omega_3)\tau_2}\;\phi^{(\mathrm{P})}_{k}(x_1)(\phi^{(\mathrm{P})}_{l}(x_1))^*\,\phi^{(\mathrm{P})}_{l+m}(x_2)(\phi^{(\mathrm{P})}_{k+m}(x_2))^*\\
&=-\frac{1}{L}\sum_m \mathfrak{U}_{m,m}\sum_{k,l}\int_{\omega_1}\int_{\omega_2}\left(-\mathrm{i}\,\omega_1+\bar\varepsilon^{(I)}_{k}\right)^{-1}\left(-\mathrm{i}\,\omega_2+\bar\varepsilon^{(I)}_{l}\right)^{-1}\left(-\mathrm{i}\,(\omega_1-\omega_2)+\bar\varepsilon^{(I)}_{k+m}-\bar\varepsilon^{(I)}_{l+m}\right)^{-1}\mathrm{e}^{-\mathrm{i}\,\omega_2(\tau_1-\tau_2)}\\
&\qquad\left(\Theta(-\bar\varepsilon^{(I)}_{k+m})\Theta(\bar\varepsilon^{(I)}_{l+m})-\Theta(\bar\varepsilon^{(I)}_{k+m})\Theta(-\bar\varepsilon^{(I)}_{l+m})\right)\,(\phi^{(\mathrm{P})}_{k}(x_2))^*\phi^{(\mathrm{P})}_{k}(x_1)(\phi^{(\mathrm{P})}_{l}(x_1))^*\phi^{(\mathrm{P})}_{l}(x_2)\,\mathrm{e}^{-\mathrm{i}\,\omega_1(\tau_2-\tau_1)}\\
&=-\frac{1}{L}\sum_m \mathfrak{U}_{m,m}\sum_{k,l}\int_{\omega_1}\left(-\mathrm{i}\,\omega_1+\bar\varepsilon^{(I)}_{k}\right)^{-1}\left(-\mathrm{i}\,\omega_1+\bar\varepsilon^{(I)}_{k+m}-\bar\varepsilon^{(I)}_{l+m}+\bar\varepsilon^{(I)}_{l}\right)^{-1}\;\mathrm{e}^{-\mathrm{i}\,\omega_1(\tau_2-\tau_1)}\\
&\qquad\left(\Theta(-\bar\varepsilon^{(I)}_{k+m})\Theta(\bar\varepsilon^{(I)}_{l+m})-\Theta(\bar\varepsilon^{(I)}_{k+m})\Theta(-\bar\varepsilon^{(I)}_{l+m})\right)\,(\phi^{(\mathrm{P})}_{k}(x_2))^*\phi^{(\mathrm{P})}_{k}(x_1)(\phi^{(\mathrm{P})}_{l}(x_1))^*\phi^{(\mathrm{P})}_{l}(x_2)\\
&\qquad\Big\{\;\mathrm{e}^{-|\bar\varepsilon^{(I)}_{l}||\tau_1-\tau_2|}\left(\Theta_\tau(\tau_1-\tau_2)\Theta(\bar\varepsilon^{(I)}_{l})-\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar\varepsilon^{(I)}_{l})\right) \qquad\text{(B.37)}\\
&\qquad-\mathrm{e}^{-|\bar\varepsilon^{(I)}_{k+m}-\bar\varepsilon^{(I)}_{l+m}||\tau_1-\tau_2|}\,\mathrm{e}^{-\mathrm{i}\,\omega_1(\tau_1-\tau_2)}\left(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar\varepsilon^{(I)}_{k+m}+\bar\varepsilon^{(I)}_{l+m})-\Theta_\tau(\tau_2-\tau_1)\Theta(\bar\varepsilon^{(I)}_{k+m}-\bar\varepsilon^{(I)}_{l+m})\right)\Big\}. \qquad\text{(B.38)}
\end{aligned}
$$

We start with line (B.37) where it is important to look at the $m=0$ term seperately:

$$
\begin{aligned}
&-\frac{1}{L}\,\mathfrak{U}_{0,0}\sum_{k,l}\int_{\omega_1}\left(-\mathrm{i}\,\omega_1+\bar\varepsilon^{(I)}_{k}\right)^{-2}\;\mathrm{e}^{-\mathrm{i}\,\omega_1(\tau_2-\tau_1)}\,\mathrm{e}^{-\bar\varepsilon^{(I)}_{l}(\tau_1-\tau_2)}\\
&\qquad\left(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar\varepsilon^{(I)}_{k})\Theta(\bar\varepsilon^{(I)}_{l})+\Theta_\tau(\tau_2-\tau_1)\Theta(\bar\varepsilon^{(I)}_{k})\Theta(-\bar\varepsilon^{(I)}_{l})\right)\,(\phi^{(\mathrm{P})}_{k}(x_2))^*\phi^{(\mathrm{P})}_{k}(x_1)(\phi^{(\mathrm{P})}_{l}(x_1))^*\phi^{(\mathrm{P})}_{l}(x_2)\\
&=-\frac{1}{L}\,\mathfrak{U}_{0,0}\sum_{k,l}\;\mathrm{e}^{\bar\varepsilon^{(I)}_{k}(\tau_1-\tau_2)}\,|\tau_1-\tau_2|\,\left(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar\varepsilon^{(I)}_{k})-\Theta_\tau(\tau_2-\tau_1)\Theta(\bar\varepsilon^{(I)}_{k})\right)\;\mathrm{e}^{-\bar\varepsilon^{(I)}_{l}(\tau_1-\tau_2)}\\
&\qquad\left(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar\varepsilon^{(I)}_{k})\Theta(\bar\varepsilon^{(I)}_{l})+\Theta_\tau(\tau_2-\tau_1)\Theta(\bar\varepsilon^{(I)}_{k})\Theta(-\bar\varepsilon^{(I)}_{l})\right)\,(\phi^{(\mathrm{P})}_{k}(x_2))^*\phi^{(\mathrm{P})}_{k}(x_1)(\phi^{(\mathrm{P})}_{l}(x_1))^*\phi^{(\mathrm{P})}_{l}(x_2)\\
&=-\frac{1}{L}\,\mathfrak{U}_{0,0}\sum_{k,l}\;\mathrm{e}^{-|\bar\varepsilon^{(I)}_{k}-\bar\varepsilon^{(I)}_{l}||\tau_1-\tau_2|}\,|\tau_1-\tau_2|\,(\phi^{(\mathrm{P})}_{k}(x_2))^*\phi^{(\mathrm{P})}_{k}(x_1)(\phi^{(\mathrm{P})}_{l}(x_1))^*\phi^{(\mathrm{P})}_{l}(x_2)\\
&\qquad\left(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar\varepsilon^{(I)}_{k})\Theta(\bar\varepsilon^{(I)}_{l})-\Theta_\tau(\tau_2-\tau_1)\Theta(\bar\varepsilon^{(I)}_{k})\Theta(-\bar\varepsilon^{(I)}_{l})\right)\\
&=-\frac{1}{L}\,\mathfrak{U}_{0,0}\sum_{k,l}\;\mathrm{e}^{-|\bar\varepsilon^{(I)}_{k}-\bar\varepsilon^{(I)}_{l}||\tau_1-\tau_2|}\,|\tau_1-\tau_2|\,(\phi^{(\mathrm{P})}_{k}(x_2))^*\phi^{(\mathrm{P})}_{k}(x_1)(\phi^{(\mathrm{P})}_{l}(x_1))^*\phi^{(\mathrm{P})}_{l}(x_2)\,\Theta(-\bar\varepsilon^{(I)}_{k})\Theta(\bar\varepsilon^{(I)}_{l}), \qquad\text{(B.39)}
\end{aligned}
$$

In the last step we interchanged the summation indices k and l in the term with $\Theta_\tau(\tau_2-\tau_1)$ which is just a relabelling of the variables and does not change the result. For odd particle numbers or $I=\mathrm{P}$ we shift the k- and l-sum so that $k\to -k$ and $l\to -l$ and, for even particle numbers or $I=\mathrm{A}$, we shift the k- and l-sum so that $k\to -k-1$ and $l\to -l-1$. We can then use Eq. (B.12) and remove the $\Theta_\tau(\tau)$-functions.

We can now put this term and the result (B.36) of the first two $\Delta^{(I)}_{\lambda=0}$-terms together:

$$
\begin{aligned}
&=-\frac{1}{L}\,\mathfrak{U}_{0,0}\sum_{k,l}\,\mathrm{e}^{-|\bar\varepsilon^{(I)}_k-\bar\varepsilon^{(I)}_l||\tau_1-\tau_2|}\,|\tau_1-\tau_2|\,(\phi^{(\mathrm{P})}_k(x_2))^*\phi^{(\mathrm{P})}_k(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\,\Theta(-\bar\varepsilon^{(I)}_k)\Theta(\bar\varepsilon^{(I)}_l)\\
&\quad+\frac{1}{L}\,\mathfrak{U}_{0,0}\sum_{k,l}\,\mathrm{e}^{-|\bar\varepsilon^{(I)}_k-\bar\varepsilon^{(I)}_l||\tau_1-\tau_2|}|\tau_1-\tau_2|\,(\phi^{(\mathrm{P})}_k(x_2))^*\phi^{(\mathrm{P})}_k(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\,\Theta(-\bar\varepsilon^{(I)}_k)\Theta(\bar\varepsilon^{(I)}_l)\\
&\quad+\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\,\mathrm{e}^{-|\bar\varepsilon^{(I)}_{k+m}-\bar\varepsilon^{(I)}_l||\tau_1-\tau_2|}|\tau_1-\tau_2|\,(\phi^{(\mathrm{P})}_{k+m}(x_2))^*\phi^{(\mathrm{P})}_{k+m}(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\\
&\qquad\Big(\Theta(-\bar\varepsilon^{(I)}_{k+m})\Theta(-\bar\varepsilon^{(I)}_k)\Theta(\bar\varepsilon^{(I)}_l)+\Theta(\bar\varepsilon^{(I)}_{k+m})\Theta(-\bar\varepsilon^{(I)}_k)\Theta(-\bar\varepsilon^{(I)}_l)\Big)\\
&=\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\,\mathrm{e}^{-|\bar\varepsilon^{(I)}_{k+m}-\bar\varepsilon^{(I)}_l||\tau_1-\tau_2|}|\tau_1-\tau_2|\,(\phi^{(\mathrm{P})}_{k+m}(x_2))^*\phi^{(\mathrm{P})}_{k+m}(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\\
&\qquad\Big(\Theta(-\bar\varepsilon^{(I)}_{k+m})\Theta(-\bar\varepsilon^{(I)}_k)\Theta(\bar\varepsilon^{(I)}_l)+\Theta(\bar\varepsilon^{(I)}_{k+m})\Theta(-\bar\varepsilon^{(I)}_k)\Theta(-\bar\varepsilon^{(I)}_l)\Big)\\
&=\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\,\mathrm{e}^{-|\bar\varepsilon^{(I)}_k-\bar\varepsilon^{(I)}_l||\tau_1-\tau_2|}|\tau_1-\tau_2|\,(\phi^{(\mathrm{P})}_k(x_2))^*\phi^{(\mathrm{P})}_k(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\\
&\qquad\Theta(-\bar\varepsilon^{(I)}_{k+m})\,\Big(\Theta(-\bar\varepsilon^{(I)}_k)\Theta(\bar\varepsilon^{(I)}_l)+\Theta(\bar\varepsilon^{(I)}_k)\Theta(-\bar\varepsilon^{(I)}_l)\Big)\,.
\end{aligned}
\tag{B.40}
$$

Here, we shifted the k-sum so that $k\to k-m$ and the m-sum so that $m\to -m$ and used $\mathfrak{U}_{m,m}\equiv\mathfrak{U}_{-m,-m}$.

Let us now discuss the evaluation of all other terms, namely the ones with $m\neq 0$, in line (B.37):

$$
\begin{aligned}
&-\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\int_{\omega_1}\Big(-\mathrm{i}\,\omega_1+\bar\varepsilon^{(I)}_k\Big)^{-1}\Big(-\mathrm{i}\,\omega_1+\bar\varepsilon^{(I)}_{k+m}-\bar\varepsilon^{(I)}_{l+m}+\bar\varepsilon^{(I)}_l\Big)^{-1}\,\mathrm{e}^{-\mathrm{i}\,\omega_1(\tau_2-\tau_1)}\\
&\quad\Big(\Theta(-\bar\varepsilon^{(I)}_{k+m})\Theta(\bar\varepsilon^{(I)}_{l+m})-\Theta(\bar\varepsilon^{(I)}_{k+m})\Theta(-\bar\varepsilon^{(I)}_{l+m})\Big)\,\Big(\Theta_\tau(\tau_1-\tau_2)\Theta(\bar\varepsilon^{(I)}_l)-\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar\varepsilon^{(I)}_l)\Big)\\
&\qquad\mathrm{e}^{-\bar\varepsilon^{(I)}_l(\tau_1-\tau_2)}\,(\phi^{(\mathrm{P})}_k(x_2))^*\phi^{(\mathrm{P})}_k(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\\
=&-\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\Big(\bar\varepsilon^{(I)}_{k+m}-\bar\varepsilon^{(I)}_{l+m}-\bar\varepsilon^{(I)}_k+\bar\varepsilon^{(I)}_l\Big)^{-1}\,\mathrm{e}^{-\bar\varepsilon^{(I)}_l(\tau_1-\tau_2)}\,(\phi^{(\mathrm{P})}_k(x_2))^*\phi^{(\mathrm{P})}_k(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\\
&\quad\Big(\Theta(-\bar\varepsilon^{(I)}_{k+m})\Theta(\bar\varepsilon^{(I)}_{l+m})-\Theta(\bar\varepsilon^{(I)}_{k+m})\Theta(-\bar\varepsilon^{(I)}_{l+m})\Big)\,\Big(\Theta_\tau(\tau_1-\tau_2)\Theta(\bar\varepsilon^{(I)}_l)-\Theta_\tau(\tau_2-\tau_1)\Theta(-\bar\varepsilon^{(I)}_l)\Big)\\
&\qquad\Big\{-\mathrm{e}^{\bar\varepsilon^{(I)}_k(\tau_1-\tau_2)}\,\Big(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar\varepsilon^{(I)}_k)-\Theta_\tau(\tau_2-\tau_1)\Theta(\bar\varepsilon^{(I)}_k)\Big)
\end{aligned}
\tag{B.41}
$$

$$
\begin{aligned}
&\qquad+\mathrm{e}^{(\epsilon_{k+m}-\epsilon_{l+m}+\epsilon_l)(\tau_1-\tau_2)}\,\Big(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar\varepsilon^{(I)}_{k+m}+\bar\varepsilon^{(I)}_{l+m}-\bar\varepsilon^{(I)}_l)-\Theta_\tau(\tau_2-\tau_1)\Theta(\bar\varepsilon^{(I)}_{k+m}-\bar\varepsilon^{(I)}_{l+m}+\bar\varepsilon^{(I)}_l)\Big)\Big\}\,.
\end{aligned}
\tag{B.42}
$$

Looking at the two terms seperately and starting with (B.41):

$$
\begin{aligned}
&\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\Big(\bar\varepsilon^{(I)}_{k+m}-\bar\varepsilon^{(I)}_{l+m}-\bar\varepsilon^{(I)}_k+\bar\varepsilon^{(I)}_l\Big)^{-1}\,\mathrm{e}^{-|\bar\varepsilon^{(I)}_k-\bar\varepsilon^{(I)}_l||\tau_1-\tau_2|}\,(\phi^{(\mathrm{P})}_k(x_2))^*\phi^{(\mathrm{P})}_k(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\\
&\qquad\Big(\Theta(-\bar\varepsilon^{(I)}_{k+m})\Theta(\bar\varepsilon^{(I)}_{l+m})-\Theta(\bar\varepsilon^{(I)}_{k+m})\Theta(-\bar\varepsilon^{(I)}_{l+m})\Big)\,\Big(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar\varepsilon^{(I)}_k)\Theta(\bar\varepsilon^{(I)}_l)+\Theta_\tau(\tau_2-\tau_1)\Theta(\bar\varepsilon^{(I)}_k)\Theta(-\bar\varepsilon^{(I)}_l)\Big)\\
=&\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\Big(\bar\varepsilon^{(I)}_{k+m}-\bar\varepsilon^{(I)}_{l+m}-\bar\varepsilon^{(I)}_k+\bar\varepsilon^{(I)}_l\Big)^{-1}\,\mathrm{e}^{-|\bar\varepsilon^{(I)}_k-\bar\varepsilon^{(I)}_l||\tau_1-\tau_2|}\,(\phi^{(\mathrm{P})}_k(x_2))^*\phi^{(\mathrm{P})}_k(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\\
&\qquad\Big(\Theta(-\bar\varepsilon^{(I)}_{k+m})\Theta(\bar\varepsilon^{(I)}_{l+m})-\Theta(\bar\varepsilon^{(I)}_{k+m})\Theta(-\bar\varepsilon^{(I)}_{l+m})\Big)\,\Theta(-\bar\varepsilon^{(I)}_k)\Theta(\bar\varepsilon^{(I)}_l)\\
=&\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\Big(\bar\varepsilon^{(I)}_{k+m}-\bar\varepsilon^{(I)}_{l+m}-\bar\varepsilon^{(I)}_k+\bar\varepsilon^{(I)}_l\Big)^{-1}\,\mathrm{e}^{-|\bar\varepsilon^{(I)}_k-\bar\varepsilon^{(I)}_l||\tau_1-\tau_2|}\,(\phi^{(\mathrm{P})}_k(x_2))^*\phi^{(\mathrm{P})}_k(x_1)(\phi^{(\mathrm{P})}_l(x_1))^*\phi^{(\mathrm{P})}_l(x_2)\\
&\qquad\Big(\Theta(-\bar\varepsilon^{(I)}_{k+m})-\Theta(-\bar\varepsilon^{(I)}_{l+m})\Big)\,\Theta(-\bar\varepsilon^{(I)}_k)\Theta(\bar\varepsilon^{(I)}_l)\,.
\end{aligned}
\tag{B.43}
$$

In the first step we interchanged the summation indices k and l which is again only a relabelling of these parameters. We then used the fact that we can shift the m-sum so that $m \to -m$ and use that $\mathfrak{U}_{m,m} \equiv \mathfrak{U}_{-m,-m}$. For odd particle numbers we shift the k- and l-sum so that $k \to -k$ and $l \to -l$ and for even particle numbers we shift the k- and l-sum so that $k \to -k-1$ and $l \to -l-1$. We then used that $\phi_k^{(\mathrm{P})}(x) \equiv (\phi_{-k}^{(\mathrm{P})}(x))^*$, $(\phi_{k-1}^{(\mathrm{P})}(x_1))^* \phi_{k-1}^{(\mathrm{P})}(x_2) \equiv (\phi_k^{(\mathrm{P})}(x_1))^* \phi_k^{(\mathrm{P})}(x_2)$ and Eq. (B.12). In the last step we used Eq. (B.9).

We come to the evaluation of line (B.42):

$$
\begin{aligned}
&-\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\Big(\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_{k}^{(I)}+\bar{\varepsilon}_{l}^{(I)}\Big)^{-1}\ \mathrm{e}^{-|\epsilon_{k+m}-\epsilon_{l+m}||\tau_1-\tau_2|}\ (\phi_k^{(\mathrm{P})}(x_2))^*\phi_k^{(\mathrm{P})}(x_1)(\phi_l^{(\mathrm{P})}(x_1))^*\phi_l^{(\mathrm{P})}(x_2)\\
&\qquad\Big(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar{\varepsilon}_{k+m}^{(I)}+\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_{l}^{(I)})\Theta(\bar{\varepsilon}_{l}^{(I)})+\Theta_\tau(\tau_2-\tau_1)\Theta(\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}+\bar{\varepsilon}_{l}^{(I)})\Theta(-\bar{\varepsilon}_{l}^{(I)})\Big)\\
&\qquad\quad\Big(\Theta(-\bar{\varepsilon}_{k+m}^{(I)})\Theta(\bar{\varepsilon}_{l+m}^{(I)})-\Theta(\bar{\varepsilon}_{k+m}^{(I)})\Theta(-\bar{\varepsilon}_{l+m}^{(I)})\Big)\\
=&-\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\Big(\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_{k}^{(I)}+\bar{\varepsilon}_{l}^{(I)}\Big)^{-1}\ \mathrm{e}^{-|\epsilon_{k+m}-\epsilon_{l+m}||\tau_1-\tau_2|}\ (\phi_k^{(\mathrm{P})}(x_2))^*\phi_k^{(\mathrm{P})}(x_1)(\phi_l^{(\mathrm{P})}(x_1))^*\phi_l^{(\mathrm{P})}(x_2)\\
&\qquad\Big(\ \Theta_\tau(\tau_1-\tau_2)\Theta(-\bar{\varepsilon}_{k+m}^{(I)})\Theta(\bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_{l}^{(I)})\Theta(-\bar{\varepsilon}_{k+m}^{(I)}+\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_{l}^{(I)})\\
&\qquad-\Theta_\tau(\tau_2-\tau_1)\Theta(\bar{\varepsilon}_{k+m}^{(I)})\Theta(-\bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_{l}^{(I)})\Theta(\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}+\bar{\varepsilon}_{l}^{(I)})\Big)\\
=&\ \ \frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\Big(\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_{k}^{(I)}+\bar{\varepsilon}_{l}^{(I)}\Big)^{-1}\ \mathrm{e}^{-|\epsilon_{k}-\epsilon_{l}||\tau_1-\tau_2|}\ (\phi_k^{(\mathrm{P})}(x_2))^*\phi_k^{(\mathrm{P})}(x_1)(\phi_l^{(\mathrm{P})}(x_1))^*\phi_l^{(\mathrm{P})}(x_2)\\
&\qquad\Big(\ \Theta_\tau(\tau_1-\tau_2)\Theta(-\bar{\varepsilon}_{k}^{(I)})\Theta(\bar{\varepsilon}_{l}^{(I)})\Theta(\bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_{k}^{(I)}+\bar{\varepsilon}_{l}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)})\\
&\qquad-\Theta_\tau(\tau_2-\tau_1)\Theta(\bar{\varepsilon}_{k}^{(I)})\Theta(-\bar{\varepsilon}_{l}^{(I)})\Theta(-\bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_{k}^{(I)}-\bar{\varepsilon}_{l}^{(I)}+\bar{\varepsilon}_{l+m}^{(I)})\Big),
\end{aligned}
\tag{B.44}
$$

where we used Eq. (B.5) in the first step and in the second step we shifted the k-sum so that $k \to k-m$, the l-sum so that $k \to l-m$ and the m-sum so that $m \to -m$ and used $\mathfrak{U}_{m,m} \equiv \mathfrak{U}_{-m,-m}$.

We continue with the calculation of line (B.38). We use Eq. (B.5) to simplify the expression before we solve the remaining ω_1-integral:

$$
\begin{aligned}
&\frac{1}{L}\sum_{m}\mathfrak{U}_{m,m}\sum_{k,l}\int_{\omega_1}\Big(-\mathrm{i}\,\omega_1+\bar{\varepsilon}_{k}^{(I)}\Big)^{-1}\Big(-\mathrm{i}\,\omega_1+\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}+\bar{\varepsilon}_{l}^{(I)}\Big)^{-1}\ \mathrm{e}^{-|\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}||\tau_1-\tau_2|}\\
&\qquad\Big(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar{\varepsilon}_{k+m}^{(I)})\Theta(\bar{\varepsilon}_{l+m}^{(I)})+\Theta_\tau(\tau_2-\tau_1)\Theta(\bar{\varepsilon}_{k+m}^{(I)})\Theta(-\bar{\varepsilon}_{l+m}^{(I)})\Big)\\
&\qquad\quad(\phi_k^{(\mathrm{P})}(x_2))^*\phi_k^{(\mathrm{P})}(x_1)(\phi_l^{(\mathrm{P})}(x_1))^*\phi_l^{(\mathrm{P})}(x_2)\\
=&\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\Big(\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_{k}^{(I)}+\bar{\varepsilon}_{l}^{(I)}\Big)^{-1}\ \mathrm{e}^{-|\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}||\tau_1-\tau_2|}\ (\phi_k^{(\mathrm{P})}(x_2))^*\phi_k^{(\mathrm{P})}(x_1)(\phi_l^{(\mathrm{P})}(x_1))^*\phi_l^{(\mathrm{P})}(x_2)\\
&\qquad\Big(\Theta(-\bar{\varepsilon}_{k+m}^{(I)}+\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_{l}^{(I)})\Theta(\bar{\varepsilon}_{k}^{(I)})-\Theta(\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}+\bar{\varepsilon}_{l}^{(I)})\Theta(-\bar{\varepsilon}_{k}^{(I)})\Big)\\
&\qquad\quad\Big(\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar{\varepsilon}_{k+m}^{(I)})\Theta(\bar{\varepsilon}_{l+m}^{(I)})+\Theta_\tau(\tau_2-\tau_1)\Theta(\bar{\varepsilon}_{k+m}^{(I)})\Theta(-\bar{\varepsilon}_{l+m}^{(I)})\Big)\\
=&-\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\Big(\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_{k}^{(I)}+\bar{\varepsilon}_{l}^{(I)}\Big)^{-1}\ \mathrm{e}^{-|\bar{\varepsilon}_{k}^{(I)}-\bar{\varepsilon}_{l}^{(I)}||\tau_1-\tau_2|}\ (\phi_k^{(\mathrm{P})}(x_2))^*\phi_k^{(\mathrm{P})}(x_1)(\phi_l^{(\mathrm{P})}(x_1))^*\phi_l^{(\mathrm{P})}(x_2)\\
&\qquad\Big(\ \Theta_\tau(\tau_1-\tau_2)\Theta(-\bar{\varepsilon}_{k}^{(I)})\Theta(\bar{\varepsilon}_{l}^{(I)})\ \Big(\Theta(-\bar{\varepsilon}_{k}^{(I)}+\bar{\varepsilon}_{l}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_{k+m}^{(I)})-\Theta(\bar{\varepsilon}_{k}^{(I)}-\bar{\varepsilon}_{l}^{(I)}+\bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_{k+m}^{(I)})\Big)\\
&\qquad+\Theta_\tau(\tau_2-\tau_1)\Theta(\bar{\varepsilon}_{k}^{(I)})\Theta(-\bar{\varepsilon}_{l}^{(I)})\ \Big(\Theta(-\bar{\varepsilon}_{k}^{(I)}+\bar{\varepsilon}_{l}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_{k+m}^{(I)})-\Theta(\bar{\varepsilon}_{k}^{(I)}-\bar{\varepsilon}_{l}^{(I)}+\bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_{k+m}^{(I)})\Big)\Big)\\
=&-\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\Big(\bar{\varepsilon}_{k+m}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)}-\bar{\varepsilon}_{k}^{(I)}+\bar{\varepsilon}_{l}^{(I)}\Big)^{-1}\ \mathrm{e}^{-|\bar{\varepsilon}_{k}^{(I)}-\bar{\varepsilon}_{l}^{(I)}||\tau_1-\tau_2|}\ (\phi_k^{(\mathrm{P})}(x_2))^*\phi_k^{(\mathrm{P})}(x_1)(\phi_l^{(\mathrm{P})}(x_1))^*\phi_l^{(\mathrm{P})}(x_2)\\
&\qquad\Big(\ \Theta_\tau(\tau_1-\tau_2)\Theta(-\bar{\varepsilon}_{k}^{(I)})\Theta(\bar{\varepsilon}_{l}^{(I)})\ \Big(\Theta(\bar{\varepsilon}_{k+m}^{(I)})-\Theta(\bar{\varepsilon}_{k}^{(I)}-\bar{\varepsilon}_{l}^{(I)}+\bar{\varepsilon}_{l+m}^{(I)})\Big)\\
&\qquad+\Theta_\tau(\tau_2-\tau_1)\Theta(\bar{\varepsilon}_{k}^{(I)})\Theta(-\bar{\varepsilon}_{l}^{(I)})\ \Big(\Theta(-\bar{\varepsilon}_{k}^{(I)}+\bar{\varepsilon}_{l}^{(I)}-\bar{\varepsilon}_{l+m}^{(I)})-\Theta(-\bar{\varepsilon}_{k+m}^{(I)})\Big)\Big)
\end{aligned}
\tag{B.45}
$$

where we excluded the term with $m = 0$ in the sums here because for this term the ω_1 integral reduces to

$$\int \frac{\mathrm{d}\omega_1}{2\pi} \left(-\mathrm{i}\,\omega_1 + \bar{\varepsilon}_k^{(I)}\right)^{-2} = 0\,. \tag{B.46}$$

In the second step we shifted the k-sum so that $k \to k - m$, the l-sum so that $k \to l - m$ and the m-sum so that $m \to -m$ and used $\mathfrak{U}_{m,m} \equiv \mathfrak{U}_{-m,-m}$. In the last step, we then used Eq. (B.9) to simplify the Θ-terms in to ways:

$$\begin{aligned}
&\Theta(-\bar{\varepsilon}_k^{(I)} + \bar{\varepsilon}_l^{(I)} - \bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_{k+m}^{(I)}) - \Theta(\bar{\varepsilon}_k^{(I)} - \bar{\varepsilon}_l^{(I)} + \bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_{k+m}^{(I)}) = \Theta(\bar{\varepsilon}_{k+m}^{(I)}) - \Theta(\bar{\varepsilon}_k^{(I)} - \bar{\varepsilon}_l^{(I)} + \bar{\varepsilon}_{l+m}^{(I)})\,,\\
&\Theta(-\bar{\varepsilon}_k^{(I)} + \bar{\varepsilon}_l^{(I)} - \bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_{k+m}^{(I)}) - \Theta(\bar{\varepsilon}_k^{(I)} - \bar{\varepsilon}_l^{(I)} + \bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_{k+m}^{(I)}) = \Theta(-\bar{\varepsilon}_k^{(I)} + \bar{\varepsilon}_l^{(I)} - \bar{\varepsilon}_{l+m}^{(I)}) - \Theta(-\bar{\varepsilon}_{k+m}^{(I)})\,.
\end{aligned} \tag{B.47}$$

Again, it will become clear now why we choose to use these two different transformations when we put this result together with (B.44):

$$\begin{aligned}
&\frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\left(\bar{\varepsilon}_{k+m}^{(I)} - \bar{\varepsilon}_{l+m}^{(I)} - \bar{\varepsilon}_k^{(I)} + \bar{\varepsilon}_l^{(I)}\right)^{-1} \mathrm{e}^{-|\bar{\varepsilon}_k^{(I)} - \bar{\varepsilon}_l^{(I)}||\tau_1-\tau_2|}\,(\phi_k^{(\mathrm{P})}(x_2))^*\phi_k^{(\mathrm{P})}(x_1)(\phi_l^{(\mathrm{P})}(x_1))^*\phi_l^{(\mathrm{P})}(x_2)\\
&\quad\Big(\;\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar{\varepsilon}_k^{(I)})\Theta(\bar{\varepsilon}_l^{(I)})\left(\Theta(\bar{\varepsilon}_{l+m}^{(I)})\Theta(-\bar{\varepsilon}_k^{(I)} + \bar{\varepsilon}_l^{(I)} - \bar{\varepsilon}_{l+m}^{(I)}) - \Theta(\bar{\varepsilon}_{k+m}^{(I)}) + \Theta(\bar{\varepsilon}_k^{(I)} - \bar{\varepsilon}_l^{(I)} + \bar{\varepsilon}_{l+m}^{(I)})\right)\\
&\quad + \Theta_\tau(\tau_2-\tau_1)\Theta(\bar{\varepsilon}_k^{(I)})\Theta(-\bar{\varepsilon}_l^{(I)})\left(-\Theta(-\bar{\varepsilon}_{l+m}^{(I)})\Theta(\bar{\varepsilon}_k^{(I)} - \bar{\varepsilon}_l^{(I)} + \bar{\varepsilon}_{l+m}^{(I)}) - \Theta(-\bar{\varepsilon}_k^{(I)} + \bar{\varepsilon}_l^{(I)} - \bar{\varepsilon}_{l+m}^{(I)}) + \Theta(-\bar{\varepsilon}_{k+m}^{(I)})\right)\Big)\\
&= \frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\left(\bar{\varepsilon}_{k+m}^{(I)} - \bar{\varepsilon}_{l+m}^{(I)} - \bar{\varepsilon}_k^{(I)} + \bar{\varepsilon}_l^{(I)}\right)^{-1} \mathrm{e}^{-|\bar{\varepsilon}_k^{(I)} - \bar{\varepsilon}_l^{(I)}||\tau_1-\tau_2|}\,(\phi_k^{(\mathrm{P})}(x_2))^*\phi_k^{(\mathrm{P})}(x_1)(\phi_l^{(\mathrm{P})}(x_1))^*\phi_l^{(\mathrm{P})}(x_2)\\
&\quad\Big(\;\Theta_\tau(\tau_1-\tau_2)\Theta(-\bar{\varepsilon}_k^{(I)})\Theta(\bar{\varepsilon}_l^{(I)})\left(\Theta(\bar{\varepsilon}_{l+m}^{(I)}) - \Theta(\bar{\varepsilon}_{k+m}^{(I)})\right)\\
&\quad + \Theta_\tau(\tau_2-\tau_1)\Theta(\bar{\varepsilon}_k^{(I)})\Theta(-\bar{\varepsilon}_l^{(I)})\left(-\Theta(-\bar{\varepsilon}_{l+m}^{(I)}) + \Theta(-\bar{\varepsilon}_{k+m}^{(I)})\right)\Big)\\
&= \frac{1}{L}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\left(\bar{\varepsilon}_{k+m}^{(I)} - \bar{\varepsilon}_{l+m}^{(I)} - \bar{\varepsilon}_k^{(I)} + \bar{\varepsilon}_l^{(I)}\right)^{-1} \mathrm{e}^{-|\bar{\varepsilon}_k^{(I)} - \bar{\varepsilon}_l^{(I)}||\tau_1-\tau_2|}\,(\phi_k^{(\mathrm{P})}(x_2))^*\phi_k^{(\mathrm{P})}(x_1)(\phi_l^{(\mathrm{P})}(x_1))^*\phi_l^{(\mathrm{P})}(x_2)\\
&\quad\Theta(-\bar{\varepsilon}_k^{(I)})\Theta(\bar{\varepsilon}_l^{(I)})\left(\Theta(-\bar{\varepsilon}_{k+m}^{(I)}) - \Theta(-\bar{\varepsilon}_{l+m}^{(I)})\right).
\end{aligned} \tag{B.48}$$

In the first step we used the fact that $\Theta(\epsilon) + \Theta(-\epsilon) = 1$ and in the second step we interchanged the summation indices k and l in the term with $\Theta_\tau(\tau_2 - \tau_1)$ which is just a relabelling of the parameters and does not change the result. For odd particle numbers or $I = \mathrm{P}$ we shift the k- and l-sum so that $k \to -k$ and $l \to -l$ and for even particle numbers or $I = \mathrm{A}$ we shift the k- and l-sum so that $k \to -k - 1$ and $l \to -l - 1$. We can then use Eqs. (B.12) and remove the $\Theta_\tau(\tau)$-functions. This result is now completely identical with (B.43).

Taking Eqs. (B.43), (B.48) and (B.40) we can assemble the complete result for $\mathscr{G}^{(4,1)}$:

$$\begin{aligned}
&\mathscr{G}^{(4,1)}(\tau_1, x_1, 0, x_2)\\
&\qquad = \frac{1}{L^2}\sum_{k,l}(\phi_{k-l}^{(P)}(x_1))^*\phi_{k-l}^{(P)}(x_2)\Bigg\{\sum_{m\neq 0}\mathfrak{U}_{m,m}\theta(-\bar{\varepsilon}_k^{(I)})\left(\theta(-\bar{\varepsilon}_{l+m}^{(I)}) - \theta(-\bar{\varepsilon}_{k+m}^{(I)})\right)|\tau_1|\mathrm{e}^{-|\varepsilon_{k+m}^{(I)} - \varepsilon_{l+m}^{(I)}||\tau_1|}\\
&\qquad\quad + 2\sum_{m\neq 0}\frac{\mathfrak{U}_{m,m}}{\varepsilon_{k+m}^{(I)} - \varepsilon_{l+m}^{(I)} + \varepsilon_l^{(I)} - \varepsilon_k^{(I)}}\theta(-\bar{\varepsilon}_k^{(I)})\theta(\bar{\varepsilon}_l^{(I)})\left(\theta(-\bar{\varepsilon}_{l+m}^{(I)}) - \theta(-\bar{\varepsilon}_{k+m}^{(I)})\right)\mathrm{e}^{-|\varepsilon_k^{(I)} - \varepsilon_l^{(I)}||\tau_1|}\Bigg\},
\end{aligned} \tag{B.49}$$

where we set $\tau_2 = 0$ for convenience.

For the calculation of the second-order correction to the ground-state density we need the result for $\mathscr{G}^{(4,1)}$ for $\tau_1 = \tau_2 = 0$:

$$\begin{aligned}
&\mathscr{G}^{(4,1)}(0, x_1, 0, x_2)\\
&\qquad = \frac{2}{L^2}\sum_{k,l}(\phi_{k-l}^{(P)}(x_1))^*\phi_{k-l}^{(P)}(x_2)\sum_{m\neq 0}\frac{\mathfrak{U}_{m,m}}{\varepsilon_{k+m}^{(I)} - \varepsilon_{l+m}^{(I)} + \varepsilon_l^{(I)} - \varepsilon_k^{(I)}}\theta(-\bar{\varepsilon}_k^{(I)})\theta(\bar{\varepsilon}_l^{(I)})\left(\theta(-\bar{\varepsilon}_{l+m}^{(I)}) - \theta(-\bar{\varepsilon}_{k+m}^{(I)})\right).
\end{aligned} \tag{B.50}$$

In our numerical calculations in Sec. 6.4 we use the a-th Fourier coefficient of $\mathscr{G}^{(4,1)}$ given by

$$\tilde{\mathscr{G}}^{(4,1)}_{a,a}(\omega) = -\frac{2}{L^2}\sum_k\sum_{m\neq 0}\mathfrak{U}_{m,m}\Big\{\theta(-\bar{\varepsilon}^{(I)}_k)\Big(\theta(-\bar{\varepsilon}^{(I)}_{k-a+m})-\theta(-\bar{\varepsilon}^{(I)}_{k+m})\Big)\frac{|\varepsilon^{(I)}_{k+m}-\varepsilon^{(I)}_{k-a+m}|^2-\omega^2}{(\omega^2+|\varepsilon^{(I)}_{k+m}-\varepsilon^{(I)}_{k-a+m}|^2)^2}$$
$$+\frac{2}{\varepsilon^{(I)}_{k+m}-\varepsilon^{(I)}_{k-a+m}+\varepsilon^{(I)}_{k-a}-\varepsilon^{(I)}_k}\theta(-\varepsilon^{(I)}_k)\theta(\varepsilon^{(I)}_{k-a})\Big(\theta(-\bar{\varepsilon}^{(I)}_{k-a+m})-\theta(-\bar{\varepsilon}^{(I)}_{k+m})\Big)\frac{|\varepsilon^{(I)}_k-\varepsilon^{(I)}_{k-a}|}{\omega^2+|\varepsilon^{(I)}_k-\varepsilon^{(I)}_{k-a}|^2}\Big\}. \tag{B.51}$$

To obtain the first-order perturbative correction of the density-density correlation function we use the results for $\mathscr{G}^{(2,1)}$ and $\mathscr{G}^{(4,1)}$ and insert them in the flow equation for $G^{(2,1)}_\lambda$:

$$\partial_\lambda G^{(2,1)}_\lambda(\tau_1,x_1,\tau_2,x_2) = -\frac{N}{L}\left(\mathscr{G}^{(2,1)}(\tau_1,x_1,\tau_2,x_2)+\mathscr{G}^{(4,1)}(\tau_1,x_1,\tau_2,x_2)\right). \tag{B.52}$$

Since $\mathscr{G}^{(2,1)}$ and $\mathscr{G}^{(4,1)}$ are not λ-dependent the leading-order correction for $G^{(2,1)}_\lambda$ reads

$$\begin{aligned}
&G^{(2,1)}_\lambda(\tau_1,x_1,0,x_2)\\
&\quad=-\lambda\frac{N}{L}\left(\mathscr{G}^{(2,1)}(\tau_1,x_1,\tau_2,x_2)+\mathscr{G}^{(4,1)}(\tau_1,x_1,\tau_2,x_2)\right)\\
&\quad=-\lambda\frac{N}{L^3}\sum_{m\neq 0}\mathfrak{U}_{m,m}(\phi^{(P)}_m(x_1))^*\phi^{(P)}_m(x_2)\Big\{\Big(\sum_k\theta(-\bar{\varepsilon}^{(I)}_k)\theta(\bar{\varepsilon}^{(I)}_{k+m})|\tau_1|\mathrm{e}^{-|\varepsilon^{(I)}_{k+m}-\varepsilon^{(I)}_k||\tau_1|}\\
&\qquad-2\sum_{k\neq l}\frac{1}{\varepsilon^{(I)}_{k+m}-\varepsilon^{(I)}_{l+m}+\varepsilon^{(I)}_l-\varepsilon^{(I)}_k}\theta(\bar{\varepsilon}^{(I)}_{k+m})\theta(-\bar{\varepsilon}^{(I)}_k)\Big(\theta(-\varepsilon^{(I)}_l)-\theta(-\varepsilon^{(I)}_{l+m})\Big)\mathrm{e}^{-|\varepsilon^{(I)}_{k+m}-\varepsilon^{(I)}_k||\tau_1|}\Big\}\\
&\qquad+\lambda\frac{N}{L^3}\sum_{k,l}(\phi^{(P)}_{k-l}(x_1))^*\phi^{(P)}_{k-l}(x_2)\Big\{\sum_{m\neq 0}\mathfrak{U}_{m,m}\theta(-\bar{\varepsilon}^{(I)}_k)\Big(\theta(-\bar{\varepsilon}^{(I)}_{l+m})-\theta(-\bar{\varepsilon}^{(I)}_{k+m})\Big)|\tau_1|\mathrm{e}^{-|\varepsilon^{(I)}_{k+m}-\varepsilon^{(I)}_{l+m}||\tau_1|}\\
&\qquad+2\sum_{m\neq 0}\mathfrak{U}_{m,m}\frac{1}{\varepsilon^{(I)}_{k+m}-\varepsilon^{(I)}_{l+m}+\varepsilon^{(I)}_l-\varepsilon^{(I)}_k}\theta(-\bar{\varepsilon}^{(I)}_k)\theta(\bar{\varepsilon}^{(I)}_l)\Big(\theta(-\bar{\varepsilon}^{(I)}_{l+m})-\theta(-\bar{\varepsilon}^{(I)}_{k+m})\Big)\mathrm{e}^{-|\varepsilon^{(I)}_k-\varepsilon^{(I)}_l||\tau_1|}\Big\}.
\end{aligned} \tag{B.53}$$

B.2 Exact Solution for Two Identical Fermions

To benchmark our approach we compare our DFT-RG reults to the exact result of the system with two identical fermions.

Let us consider two identical particles in a finite box interacting via a two-body potential U:

$$\hat{H} = \frac{\hat{p}_1^2}{2}+\frac{\hat{p}_2^2}{2}+U(x_1-x_2) \tag{B.54}$$
$$= -\frac{1}{2}\frac{\partial^2}{\partial x_1^2}-\frac{1}{2}\frac{\partial^2}{\partial x_2^2}+U(x_1-x_2), \tag{B.55}$$

where we set $m_1 = m_2 = 1$ for the masses.

We can now construct a two-particle basis and diagonalize the problem in this two-body Hilbert space. Since we have an even number of identical fermions here, namely two, we assume a box with antiperiodic boundary conditions. Therefore, we use the one-particle basis set $\{\phi^{(\mathrm{A})}_n\}$, with $n\in\mathbb{Z}$, where the basis states $\phi^{(\mathrm{A})}_n$ are defined in Eq. (5.4).

Since we study identical fermions each state can only be occupied by a single fermion. The wavefunction for a two-body state where one fermion occupies state n_1 and the other fermion occupies state n_2 is given by a Slater determinant:

$$\varphi_{n_1 n_2}(x_1, x_2) = \frac{1}{\sqrt{2}} \begin{vmatrix} \phi^{(\mathrm{A})}_{n_1}(x_1) & \phi^{(\mathrm{A})}_{n_2}(x_1) \\ \phi^{(\mathrm{A})}_{n_1}(x_2) & \phi^{(\mathrm{A})}_{n_2}(x_2) \end{vmatrix} \tag{B.56}$$

$$= \frac{1}{\sqrt{2}} \left(\phi^{(\mathrm{A})}_{n_1}(x_1)\, \phi^{(\mathrm{A})}_{n_2}(x_2) - \phi^{(\mathrm{A})}_{n_2}(x_1)\, \phi^{(\mathrm{A})}_{n_1}(x_2) \right). \tag{B.57}$$

The two-body states $\varphi_{n_1 n_2}(x_1, x_2)$ and $\varphi_{n_2 n_1}(x_1, x_2)$ are linear-dependent states

$$\varphi_{n_1 n_2}(x_1, x_2) = -\varphi_{n_2 n_1}(x_1, x_2) \tag{B.58}$$

and therefore we only use states with $n_1 < n_2$ to construct the basis

$$\mathscr{B} := \left\{ \varphi_{n_1 n_2}(x_1, x_2) \,|\, n_1 < n_2\,,\ n_1 \in \mathbb{Z}\,,\ n_2 \in \mathbb{Z} \right\}. \tag{B.59}$$

A general two-body state can then be written as follows:

$$\psi(x_1, x_2) = \sum_{n_1 < n_2} c_{n_1 n_2}\, \varphi_{n_1 n_2}(x_1, x_2). \tag{B.60}$$

Since we have a box with finite extent here, we can count the basis states $\varphi_{n_1 n_2}$ and assign a single index to them as follows:

$$\varphi_n(x_1, x_2) := \varphi_{n_1 n_2}(x_1, x_2). \tag{B.61}$$

Thus, we have

$$\psi(x_1, x_2) = \sum_n c_n\, \varphi_n(x_1, x_2). \tag{B.62}$$

We can now diagonalize the Hamiltonian with this basis

$$\mathscr{B}' := \left\{ \varphi_n(x_1, x_2) \,|\, n \in \mathbb{Z} \right\}, \tag{B.63}$$

which yields the matrix elements

$$H_{m,n} = \left\langle \varphi_m \left| \hat{H} \right| \varphi_n \right\rangle = \int_{x_1} \int_{x_2} \varphi^*_m(x_1, x_2)\, H\, \varphi_n(x_1, x_2). \tag{B.64}$$

These matrix elements can be separated in a kinetic part and an interaction part. For example, for the matrix elements of the interaction, we find

$$\begin{aligned}
\left\langle \varphi_m \left| \hat{U} \right| \varphi_n \right\rangle &= \int_{x_1} \int_{x_2} \varphi^*_m(x_1, x_2)\, U(x_1 - x_2)\, \varphi_n(x_1, x_2) \\
&= \int_{x_1} \int_{x_2} \varphi^*_{m_1 m_2}(x_1, x_2)\, U(x_1 - x_2)\, \varphi_{n_1 n_2}(x_1, x_2) \\
&= \int_{x_1} \int_{x_2} \Big\{ (\phi^{(\mathrm{A})}_{m_1}(x_1))^* (\phi^{(\mathrm{A})}_{m_2}(x_2))^*\, U(x_1 - x_2)\, \phi^{(\mathrm{A})}_{n_1}(x_1)\, \phi^{(\mathrm{A})}_{n_2}(x_2) \\
&\qquad - (\phi^{(\mathrm{A})}_{m_1}(x_1))^* (\phi^{(\mathrm{A})}_{m_2}(x_2))^*\, U(x_1 - x_2)\, \phi^{(\mathrm{A})}_{n_2}(x_1)\, \phi^{(\mathrm{A})}_{n_1}(x_2) \\
&\qquad - (\phi^{(\mathrm{A})}_{m_2}(x_1))^* (\phi^{(\mathrm{A})}_{m_1}(x_2))^*\, U(x_1 - x_2)\, \phi^{(\mathrm{A})}_{n_1}(x_1)\, \phi^{(\mathrm{A})}_{n_2}(x_2) \\
&\qquad + (\phi^{(\mathrm{A})}_{m_2}(x_1))^* (\phi^{(\mathrm{A})}_{m_1}(x_2))^*\, U(x_1 - x_2)\, \phi^{(\mathrm{A})}_{n_2}(x_1)\, \phi^{(\mathrm{A})}_{n_1}(x_2) \Big\} \\
&= \frac{1}{L} \int_{x_1} \int_{x_2} \Big\{ (\phi^{(\mathrm{P})}_{m_1 - n_1}(x_1))^*\, U(x_1 - x_2)\, \phi^{(\mathrm{P})}_{n_2 - m_2}(x_2) \\
&\qquad - (\phi^{(\mathrm{P})}_{m_1 - n_2}(x_1))^*\, U(x_1 - x_2)\, \phi^{(\mathrm{P})}_{n_1 - m_2}(x_2) \\
&\qquad - (\phi^{(\mathrm{P})}_{m_2 - n_1}(x_1))^*\, U(x_1 - x_2)\, \phi^{(\mathrm{P})}_{n_2 - m_1}(x_2) \\
&\qquad + (\phi^{(\mathrm{P})}_{m_2 - n_2}(x_1))^*\, U(x_1 - x_2)\, \phi^{(\mathrm{P})}_{n_1 - m_1}(x_2) \Big\} \\
&= \frac{g}{L} \left(\mathfrak{U}_{m_1 - n_1, n_2 - m_2} - \mathfrak{U}_{m_1 - n_2, n_1 - m_2} - \mathfrak{U}_{m_2 - n_1, n_2 - m_1} + \mathfrak{U}_{m_2 - n_2, n_1 - m_1} \right),
\end{aligned} \tag{B.65}$$

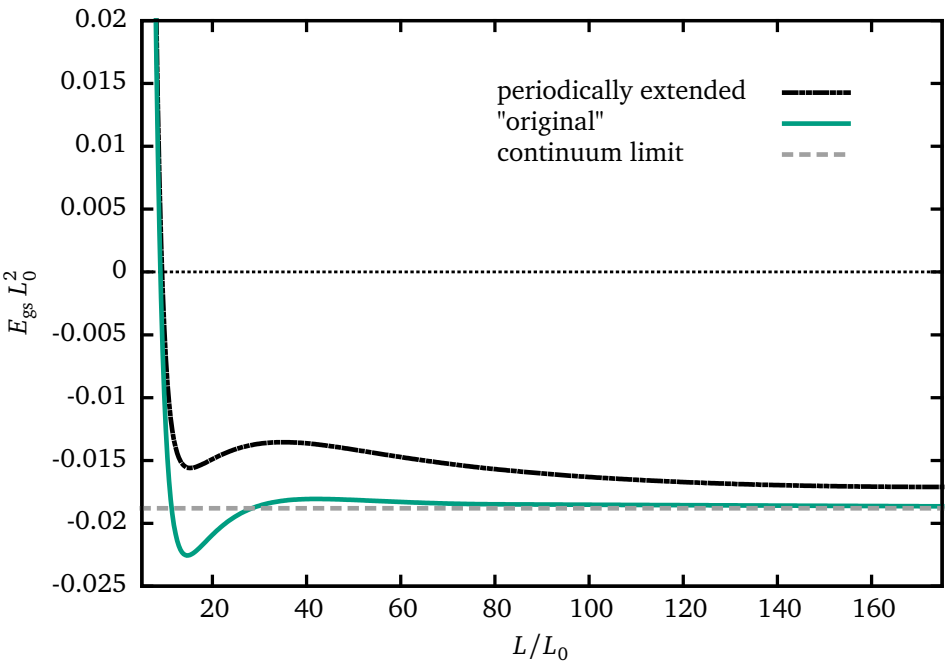

Figure B.1.: Ground-state energy of the two-body problem as a function of the extent of the box as obtained by the "original" potential and the periodically extended potential.

where we used the Fourier representation of the interaction potential (5.5). From the latter we can obtain the result for the periodically extended potential by only using the diagonal elements $\mathfrak{U}_{k,k}$, see also Eq. (5.6).

The *Schrödinger* equation for the Hamiltonian (B.55)

$$\hat{H}\,|\psi\rangle = \epsilon\,|\psi\rangle \tag{B.66}$$

can then be solved by inserting a suitably chosen $\mathbb{1}_2$-operator for the two-body problem

$$\mathbb{1}_2 = \sum_n |\varphi_n\rangle\,\langle\varphi_n|\,. \tag{B.67}$$

We then find

$$\langle\varphi_m|\hat{H}\sum_n|\varphi_n\rangle\langle\varphi_n|\psi\rangle = \epsilon\,\langle\varphi_m|\psi\rangle \tag{B.68}$$

$$\Rightarrow \sum_n H_{m,n}\,c_n = \epsilon\,c_m \tag{B.69}$$

From the solution of this system, we obtain eigenvalues for the energies and associated eigenvectors. The lowest eigenvalue ϵ_0 is equal to the ground-state energy E_{gs} of the system and the ground-state wavefunction $\Psi_{gs}(x_1, x_2)$ can be reconstructed from the eigenvector $\vec{c}_0$ corresponding to the eigenvalue ϵ_0.

In Fig. B.1, we show the results for the ground-state energy from the "original" finite-volume potential and from the periodically extended version of the potential. Clearly, our *redefined* interaction potential is not identical to the original interaction in the presence of the box. However, we observe here that the redefined potential approaches the original interaction potential in the infinite-volume limit which is of most relevance for a study of the formation of selfbound states in the absence of this auxiliary fermion-confining box. We would also like to mention that the results for both potentials approach the continuum-limit result from above.

The ground-state density can be obtained from Ψ_{gs} using Eq. (3.40):

$$n_{gs}(x) = 2 \int_{x_2} |\Psi_{gs}(x, x_2)|^2 \,. \tag{B.70}$$

The correlation function $Z^{(2)}$ follows from Eq. (3.42),

$$Z^{(2)}(0, x_1, 0, x_2) = n_{gs}(x_1)\, \delta(x_1 - x_2) + 2\, |\Psi_{gs}(x_1, x_2)|^2 \,, \tag{B.71}$$

and the density-density correlation function $G^{(2)}$ can be obtained using Eq. (3.41):

$$\begin{aligned} G^{(2)}(0, x_1, 0, x_2) &= Z^{(2)}(0, x_1, 0, x_2) - n_{gs}(x_1)\, n_{gs}(x_2) \\ &= n_{gs}(x_1)\, \delta(x_1 - x_2) + 2\, |\Psi_{gs}(x_1, x_2)|^2 - n_{gs}(x_1)\, n_{gs}(x_2) \,. \end{aligned} \tag{B.72}$$

The intrinsic density or the absolut square of the relative wavefunction (3.53) is given by

$$|\varphi_{N=2,\lambda}(r)|^2 = 2 \int_{-\frac{L-|r|}{2}}^{\frac{L-|r|}{2}} \mathrm{d}R\, |\Psi_{gs,\lambda}(R + \tfrac{1}{2}|r|, R - \tfrac{1}{2}|r|)|^2 \,. \tag{B.73}$$

C Spin-$1/2$ Fermions in a Box

In this appendix calculate the leading order perturbative correction of the density-density correlation function $G^{(2,1)}_{\lambda,\uparrow\downarrow}$ and give the next-to perturbative correction for systems of spin-$1/2$ fermions.

Moreover, we want to derive the exact result for the 1+1-fermion system with one spin-up and one spin-down fermion.

C.1 Leading-Order Perturbative Correction to the Density-Density Correlation Function

We calculate the leading-order perturbative correction to the density-density correlation function $G^{(2,1)}_{\lambda,\uparrow\downarrow}$, which is needed to calculate the second-order perturbative correction to the ground-state energy. To obtain the leading-order correction for $G^{(2,1)}_{\lambda,\uparrow\downarrow}$ we need to replace the full correlation functions $G^{(2)}_{\lambda,\sigma_1\sigma_2}$ by their initial conditions $G^{(2,0)}_{\sigma_1\sigma_2}$ in the flow equation. Since for the calculation of the energy only the results for $\tau_1 = \tau_2 = 0$ are needed we restrict our calculations to this term.

$$\partial_\lambda G^{(2,1)}_{\lambda,\uparrow\downarrow}(0,x_1,0,x_2) = -\frac{N}{L}\int_{\tau_3}\int_{x_3}\int_{x_4} G^{(2,0)}_{\uparrow\uparrow}(0,x_1,\tau_3,x_3)\,\mathfrak{U}(x_3-x_4)\,G^{(2,0)}_{\downarrow\downarrow}(\tau_3,x_4,0,x_2)\,. \tag{C.1}$$

Since the initial conditions do not depend on λ we find

$$\begin{aligned}
&G^{(2,1)}_{\lambda,\uparrow\downarrow}(0,x_1,0,x_2)\\
&\quad= -\lambda\frac{N}{L}\int_{\tau_3}\int_{x_3}\int_{x_4} G^{(2,0)}_{\uparrow\uparrow}(0,x_1,\tau_3,x_3)\,\mathfrak{U}(x_3-x_4)\,G^{(2,0)}_{\downarrow\downarrow}(\tau_3,x_4,0,x_2)\\
&\quad= -\lambda\frac{N}{L}\int_{\tau_3}\int_{x_3}\int_{x_4}\sum_m \mathfrak{U}_{m,m}\,(\phi^{(\mathrm{P})}_m(x_3))^*\phi^{(\mathrm{P})}_m(x_4)\;\Delta^{(I_\uparrow)}_{\lambda=0,\uparrow}(0,x_1,\tau_3,x_3)\,\Delta^{(I_\uparrow)}_{\lambda=0,\uparrow}(\tau_3,x_3,0,x_1)\\
&\qquad\qquad \Delta^{(I_\downarrow)}_{\lambda=0,\downarrow}(\tau_3,x_4,0,x_2)\,\Delta^{(I_\downarrow)}_{\lambda=0,\downarrow}(0,x_2,\tau_3,x_4)\\
&\quad= -\lambda\frac{N}{L}\int_{\tau_3}\int_{x_3}\int_{x_4}\sum_m \mathfrak{U}_{m,m}\,(\phi^{(\mathrm{P})}_m(x_3))^*\phi^{(\mathrm{P})}_m(x_4)\sum_{k_1\dots k_4}\int_{\omega_1}\cdots\int_{\omega_4}\left(-\mathrm{i}\,\omega_1+\bar\varepsilon^{(I_\uparrow)}_{\uparrow,k_1}\right)^{-1}\left(-\mathrm{i}\,\omega_2+\bar\varepsilon^{(I_\uparrow)}_{\uparrow,k_2}\right)^{-1}\\
&\qquad\qquad \left(-\mathrm{i}\,\omega_3+\bar\varepsilon^{(I_\downarrow)}_{\downarrow,k_3}\right)^{-1}\left(-\mathrm{i}\,\omega_4+\bar\varepsilon^{(I_\downarrow)}_{\downarrow,k_4}\right)^{-1}\;\mathrm{e}^{\mathrm{i}\,\omega_1\,\tau_3}\,\mathrm{e}^{-\mathrm{i}\,\omega_2\,\tau_3}\,\mathrm{e}^{-\mathrm{i}\,\omega_3\,\tau_3}\,\mathrm{e}^{\mathrm{i}\,\omega_4\,\tau_3}\\
&\qquad\qquad (\phi^{(I_\uparrow)}_{k_1}(x_1))^*\phi^{(I_\uparrow)}_{k_1}(x_3)\,(\phi^{(I_\uparrow)}_{k_2}(x_3))^*\phi^{(I_\uparrow)}_{k_2}(x_1)\,(\phi^{(I_\downarrow)}_{k_3}(x_4))^*\phi^{(I_\downarrow)}_{k_3}(x_2)\,(\phi^{(I_\downarrow)}_{k_4}(x_2))^*\phi^{(I_\downarrow)}_{k_4}(x_4)\\
&\quad= -\lambda\frac{N}{L}\sum_m \mathfrak{U}_{m,m}\sum_{k_1\dots k_4}\int_{\omega_1}\cdots\int_{\omega_4}\left(-\mathrm{i}\,\omega_1+\bar\varepsilon^{(I_\uparrow)}_{\uparrow,k_1}\right)^{-1}\left(-\mathrm{i}\,\omega_2+\bar\varepsilon^{(I_\uparrow)}_{\uparrow,k_2}\right)^{-1}\left(-\mathrm{i}\,\omega_3+\bar\varepsilon^{(I_\downarrow)}_{\downarrow,k_3}\right)^{-1}\left(-\mathrm{i}\,\omega_4+\bar\varepsilon^{(I_\downarrow)}_{\downarrow,k_4}\right)^{-1}\\
&\qquad\qquad \frac{\delta_{k_2+m,k_1}}{\sqrt{L}}\,\frac{\delta_{k_4+m,k_3}}{\sqrt{L}}\;2\pi\,\delta(\omega_1-\omega_2-\omega_3+\omega_4)\,(\phi^{(\mathrm{P})}_{k_1}(x_1))^*\,\phi^{(\mathrm{P})}_{k_2}(x_1)\,\phi^{(\mathrm{P})}_{k_3}(x_2)\,(\phi^{(\mathrm{P})}_{k_4}(x_2))^*\\
&\quad= -\lambda\frac{N}{L^3}\sum_m \mathfrak{U}_{m,m}\sum_{k,l}\int_{\omega_1}\cdots\int_{\omega_3}\left(-\mathrm{i}\,\omega_1+\bar\varepsilon^{(I_\uparrow)}_{\uparrow,k+m}\right)^{-1}\left(-\mathrm{i}\,\omega_2+\bar\varepsilon^{(I_\uparrow)}_{\uparrow,k}\right)^{-1}\left(-\mathrm{i}\,\omega_3+\bar\varepsilon^{(I_\downarrow)}_{\downarrow,l+m}\right)^{-1}\\
&\qquad\qquad \left(\mathrm{i}(\omega_1-\omega_2-\omega_3)+\bar\varepsilon^{(I_\downarrow)}_{\downarrow,l}\right)^{-1}\;(\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\,,
\end{aligned} \tag{C.2}$$

where we plugged in the definition for $\Delta^{(I_\sigma)}_{\lambda=0,\sigma}$ given in Eq. (5.11) and introduced the shorthand $\int_\omega = \int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}$. We also used the relation $(\phi^{(\mathrm{A})}_k(x))^*\phi^{(\mathrm{A})}_l(x) = (\phi^{(\mathrm{P})}_k(x))^*\phi^{(\mathrm{P})}_l(x)$ for the anti-periodic one-particle eigenstates.

Now we evaluate the ω integrals:

$$
\begin{aligned}
&G^{(2,1)}_{\lambda,\uparrow\downarrow}(0,x_1,0,x_2)\\
&\quad=-\lambda\frac{N}{L^3}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\int_{\omega_1}\int_{\omega_2}\left(-\mathrm{i}\,\omega_1+\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k+m}\right)^{-1}\left(-\mathrm{i}\,\omega_2+\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k}\right)^{-1}\left(\mathrm{i}(\omega_1-\omega_2)+\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l}-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m}\right)^{-1}\\
&\qquad\left(\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l})-\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l})\right)\,(\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\quad=-\lambda\frac{N}{L^3}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\int_{\omega_1}\left(-\mathrm{i}\,\omega_1+\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k+m}\right)^{-1}\left(\mathrm{i}\,\omega_1+\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l}-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m}-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k}\right)^{-1}\\
&\qquad\left(\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l}+\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m})-\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l}-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m})\right)\\
&\qquad\left(\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l})-\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l})\right)\,(\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\quad=-\lambda\frac{N}{L^3}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\left(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l}-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m}-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k}+\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k+m}\right)^{-1}\,(\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\left(\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k+m})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l}-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m}-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k})-\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k+m})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l}+\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m}+\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k})\right)\\
&\qquad\left(\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l})+\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l})\right)\\
&\quad=-\lambda\frac{N}{L^3}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\left(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l}-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m}-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k}+\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k+m}\right)^{-1}\,(\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\left(\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k+m})\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l})-\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k+m})\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l})\right)\\
&\quad=-2\lambda\frac{N}{L^3}\sum_{m\neq 0}\mathfrak{U}_{m,m}\sum_{k,l}\left(\varepsilon^{(I_\downarrow)}_{l}-\varepsilon^{(I_\downarrow)}_{l+m}-\varepsilon^{(I_\uparrow)}_{k}+\varepsilon^{(I_\uparrow)}_{k+m}\right)^{-1}\,(\phi^{(\mathrm{P})}_m(x_1))^*\,\phi^{(\mathrm{P})}_m(x_2)\\
&\qquad\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k+m})\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l}),
\end{aligned}
\tag{C.3}
$$

where we excluded the zero in the m sum because the term $\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l})-\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l+m})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,l})$ is equal to zero for $m=0$. Moreover, we used the following relations:

$$
\begin{aligned}
&\Theta(\bar{\varepsilon}^{(I_\sigma)}_{\sigma,k}-\bar{\varepsilon}^{(I_{\sigma'})}_{\sigma',l})\Theta(\bar{\varepsilon}^{(I_\sigma)}_{\sigma,k})\Theta(-\bar{\varepsilon}^{(I_{\sigma'})}_{\sigma',l})=\Theta(\bar{\varepsilon}^{(I_\sigma)}_{\sigma,k})\Theta(-\bar{\varepsilon}^{(I_{\sigma'})}_{\sigma',l})\\
&\Theta(\bar{\varepsilon}^{(I_\sigma)}_{\sigma,k}-\bar{\varepsilon}^{(I_{\sigma'})}_{\sigma',l})\Theta(-\bar{\varepsilon}^{(I_\sigma)}_{\sigma,k})\Theta(\bar{\varepsilon}^{(I_{\sigma'})}_{\sigma',l})=0\,.
\end{aligned}
\tag{C.4}
$$

In the last step we shifted the sums for the second term. For odd particle numbers or $I_\sigma=\mathrm{P}$ the shift is $k\to -k-m$ and for even particle numbers or $I_\sigma=\mathrm{A}$ the shift is $k\to -k-m-1$. We can then use the following equations here:

$$
\begin{aligned}
\bar{\varepsilon}^{(\mathrm{P})}_{\sigma,k}&=\bar{\varepsilon}^{(\mathrm{P})}_{\sigma,-k}\,,\\
\bar{\varepsilon}^{(\mathrm{A})}_{\sigma,k}&=\bar{\varepsilon}^{(\mathrm{A})}_{\sigma,-k-1}\,.
\end{aligned}
\tag{C.5}
$$

C.2 Next-to-Leading-Order Perturbative Correction to the Density-Density Correlation Function

Here, we we give the result for the next-to-leading-order perturbative correction to the density-density correlation function $G^{(2)}_{\lambda,\uparrow\downarrow}$ for the contact interaction. This term is needed to calculate the third-order perturbative correction to the ground-state energy. Moreover, we would like to use this result to improve our DFT-RG result, see our discussion in Sec. 7.3.

In Sec. 7.2 we already derived the following expression for $G^{(2,2)}_{\lambda,\uparrow\downarrow}(0,x_1,0,x_2)$, see Eq. (7.22):

$$
\begin{aligned}
&G^{(2,2)}_{\lambda,\uparrow\downarrow}(0,x_1,0,x_2)\\
&\quad=\lambda^2\left(\frac{N}{L}\right)^2\int_{\tau_3}\int_{x_3}\int_{x_4}\mathfrak{U}(x_3-x_4)\int_{\tau_5}\int_{x_5}\int_{x_6}G^{(3,0)}_{\uparrow\uparrow\uparrow}(\tau_3,x_3,0,x_1,\tau_5,x_5)\,\mathfrak{U}(x_5-x_6)\,G^{(3,0)}_{\downarrow\downarrow\downarrow}(\tau_5,x_6,\tau_3,x_4,0,x_2)\,.
\end{aligned}
\tag{C.6}
$$

From this expression we can straightforwardly calculate the next-to-leading-order perturbative correction to the density-density correlation function. The calculation of the latter is teadious, but can be in principle performed in the same way as the calculation of the leading-corrections of the density-density correlation functions in Apps. B.1 and C.1.

We find

$$
\begin{aligned}
&G^{(2,2)}_{\lambda,\uparrow\downarrow}(0,x_1,0,x_2)\\
&\quad= 2\frac{\lambda^2}{L^2}\left(\frac{N}{L}\right)^2 \sum_{k_1,\ldots,k_4} (\phi^{(\mathrm{P})}_{k_2}(x_2))^* \phi^{(\mathrm{P})}_{k_2}(x_1) (\phi^{(\mathrm{P})}_{k_3}(x_1))^* \phi^{(\mathrm{P})}_{k_3}(x_2)\\
&\qquad\Bigg\{ -2\left(\varepsilon^{(I_\uparrow)}_{k_2} - \varepsilon^{(I_\uparrow)}_{k_3} + \varepsilon^{(I_\downarrow)}_{k_1-k_2+k_4} - \varepsilon^{(I_\downarrow)}_{k_1-k_3+k_4}\right)^{-1} \left(\varepsilon^{(I_\uparrow)}_{k_1} - \varepsilon^{(I_\uparrow)}_{k_2} + \varepsilon^{(I_\downarrow)}_{k_4} - \varepsilon^{(I_\downarrow)}_{k_1-k_2+k_4}\right)^{-1}\\
&\qquad\qquad \Big[\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_1})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_4})\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_2})\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_3})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_2+k_4})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_3+k_4})\\
&\qquad\qquad\quad + \Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_1})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_4})\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_2})\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_3})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_2+k_4})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_3+k_4})\Big]\\
&\qquad + \left(\varepsilon^{(I_\uparrow)}_{k_1} - \varepsilon^{(I_\uparrow)}_{k_2} + \varepsilon^{(I_\downarrow)}_{k_4} - \varepsilon^{(I_\downarrow)}_{k_1-k_2+k_4}\right)^{-1} \left(\varepsilon^{(I_\uparrow)}_{k_1} - \varepsilon^{(I_\uparrow)}_{k_3} + \varepsilon^{(I_\downarrow)}_{k_4} - \varepsilon^{(I_\downarrow)}_{k_1-k_3+k_4}\right)^{-1}\\
&\qquad\qquad \Big[\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_1})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_4})\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_2})\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_3})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_2+k_4})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_3+k_4})\\
&\qquad\qquad\quad + \Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_1})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_4})\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_2})\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_3})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_2+k_4})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_3+k_4})\Big]\\
&\qquad + 2\left(\varepsilon^{(I_\uparrow)}_{k_2} - \varepsilon^{(I_\uparrow)}_{k_3} - \varepsilon^{(I_\downarrow)}_{k_1-k_2+k_4} + \varepsilon^{(I_\downarrow)}_{k_1-k_3+k_4}\right)^{-1} \left(\varepsilon^{(I_\uparrow)}_{k_1} - \varepsilon^{(I_\uparrow)}_{k_2} - \varepsilon^{(I_\downarrow)}_{k_4} + \varepsilon^{(I_\downarrow)}_{k_1-k_2+k_4}\right)^{-1}\\
&\qquad\qquad \Big[\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_1})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_4})\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_2})\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_3})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_2+k_4})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_3+k_4})\\
&\qquad\qquad\quad + \Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_1})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_4})\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_2})\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_3})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_2+k_4})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_3+k_4})\Big]\\
&\qquad - \left(\varepsilon^{(I_\uparrow)}_{k_1} - \varepsilon^{(I_\uparrow)}_{k_2} - \varepsilon^{(I_\downarrow)}_{k_4} + \varepsilon^{(I_\downarrow)}_{k_1-k_2+k_4}\right)^{-1} \left(\varepsilon^{(I_\uparrow)}_{k_1} - \varepsilon^{(I_\uparrow)}_{k_3} - \varepsilon^{(I_\downarrow)}_{k_4} + \varepsilon^{(I_\downarrow)}_{k_1-k_3+k_4}\right)^{-1}\\
&\qquad\qquad \Big[\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_1})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_4})\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_2})\Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_3})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_2+k_4})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_3+k_4})\\
&\qquad\qquad\quad + \Theta(-\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_1})\Theta(\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_4})\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_2})\Theta(\bar{\varepsilon}^{(I_\uparrow)}_{\uparrow,k_3})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_2+k_4})\Theta(-\bar{\varepsilon}^{(I_\downarrow)}_{\downarrow,k_1-k_3+k_4})\Big]\Bigg\}. \qquad \text{(C.7)}
\end{aligned}
$$

For the system with one spin-up and one spin-down fermion, we find

$$
\begin{aligned}
&G^{(2,2)}_{\lambda,\uparrow\downarrow}(0,x_1,0,x_2)\\
&\quad= \frac{\lambda^2}{L^3}\left(\frac{N}{L}\right)^2 \sum_{k_1\neq 0}\sum_{k_3\neq 0} \frac{1}{\varepsilon^{(\mathrm{P})}_{k_1}}\frac{1}{\varepsilon^{(\mathrm{P})}_{k_3}} (\phi^{(\mathrm{P})}_{k_3}(x_1))^* \phi^{(\mathrm{P})}_{k_3}(x_2)\\
&\quad\quad - \frac{\lambda^2}{L^3}\left(\frac{N}{L}\right)^2 \sum_{k_2\neq 0} \frac{1}{(\varepsilon^{(\mathrm{P})}_{k_2})^2} (\phi^{(\mathrm{P})}_{k_2}(x_2))^* \phi^{(\mathrm{P})}_{k_2}(x_1)\\
&\quad\quad + \frac{\lambda^2}{2L^2}\left(\frac{N}{L}\right)^2 \sum_{k_2\neq 0}\sum_{k_3\neq 0} \frac{1}{\varepsilon^{(\mathrm{P})}_{k_2}}\frac{1}{\varepsilon^{(\mathrm{P})}_{k_3}} (\phi^{(\mathrm{P})}_{k_2}(x_2))^* \phi^{(\mathrm{P})}_{k_2}(x_1) (\phi^{(\mathrm{P})}_{k_3}(x_1))^* \phi^{(\mathrm{P})}_{k_3}(x_2)\\
&\quad\quad - \frac{\lambda^2}{2L^4}\left(\frac{N}{L}\right)^2 \sum_{k_1\neq 0} \frac{1}{(\varepsilon^{(\mathrm{P})}_{k_1})^2}. \qquad \text{(C.8)}
\end{aligned}
$$

C.3 Exact Solution for 1+1-Fermions

To benchmark our approach we compare our DFT-RG results to the exact result of the system with one spin-up fermion and one spin-down fermion.

Let us consider two fermions with different spin in a finite box interacting via a contact interaction:

$$\hat{H} = \frac{\hat{p}_1^2}{2} + \frac{\hat{p}_2^2}{2} + g\,\delta(\hat{x}_1 - \hat{x}_2) \tag{C.9}$$

$$= -\frac{1}{2}\frac{\partial^2}{\partial x_1^2} - \frac{1}{2}\frac{\partial^2}{\partial x_2^2} + g\,\delta(x_1 - x_2)\,, \tag{C.10}$$

where we set $m_1 = m_2 = 1$ for the masses. In the center-of-mass frame we can decompose the Hamiltonian (C.10) into a relative and a center-of-mass part:

$$\hat{H} = \hat{H}_{\mathrm{cm}} + \hat{H}_{\mathrm{rel}}\,, \tag{C.11}$$

where

$$\hat{H}_{\mathrm{cm}} = \frac{\hat{P}^2}{2} \quad \text{and} \quad \hat{H}_{\mathrm{rel}} = \hat{p}^2 + g\,\delta(\hat{x})\,. \tag{C.12}$$

The center-of-mass momentum $\hat{P}$ and the relative momentum $\hat{p}$ are given by:

$$\hat{P} = \hat{p}_1 + \hat{p}_2 \quad \text{and} \quad \hat{p} = \frac{\hat{p}_1 - \hat{p}_2}{2}\,. \tag{C.13}$$

In this thesis, we choose to use periodic boundary conditions for a system with one spin-up and one spin-down fermion for both fermions, see also the discussion of the setup of the box in Sec. 5.1. Within Sec. 5.1 we also introduced a periodically extended potential in the box. With this, we find for the relative Hamiltonian:

$$\hat{H}_{\mathrm{rel}} = \hat{p}^2 + g \sum_{n=-\infty}^{\infty} \delta(\hat{x} + n\,L)\,, \tag{C.14}$$

where $n \in \mathbb{Z}$.

To solve the eigenvalue problem

$$\hat{H}_{\mathrm{rel}}\,\psi(x) = E\,\psi(x) \tag{C.15}$$

we use the ansatz

$$\psi(x) = \sum_m c_m\,\phi_m^{(\mathrm{P})}(x)\,, \tag{C.16}$$

where $\phi_m^{(\mathrm{P})}(x)$ are the eigenstates of a box with periodic boundary conditions defined in Eq. (5.4). Plugging Eq. (C.16) into Eq. (C.15) we find

$$\sum_m c_m\,(2\,\varepsilon_m^{(\mathrm{P})} - E)\,\phi_m^{(\mathrm{P})}(x) + g \sum_n \delta(\hat{x} + n\,L) \sum_m c_m \phi_m^{(\mathrm{P})}(x) = 0\,. \tag{C.17}$$

We multiply this equation with $(\phi_{m'}^{(\mathrm{P})}(x))^*$ and integrate over x. After relabelling $m' \leftrightarrow m$ we obtain the following equation:

$$c_m\,(2\,\varepsilon_m^{(\mathrm{P})} - E) + g \sum_n c_n\,(\phi_m^{(\mathrm{P})}(0))^* \phi_n^{(\mathrm{P})}(0) = 0\,. \tag{C.18}$$

Using the ansatz

$$c_m = A \frac{(\phi_m^{(\mathrm{P})}(0))^*}{2\,\varepsilon_m^{(\mathrm{P})} - E}\,, \tag{C.19}$$

where A is a constant, we eventually find

$$\frac{1}{L}\sum_m \frac{1}{2\,\varepsilon_m^{(\mathrm{P})} - E} = -\frac{\cot\left(\frac{\sqrt{E}\,L}{2}\right)}{2\,\sqrt{E}} = -\frac{1}{g}\,. \tag{C.20}$$

This yields an implicit equation for the calculation of the ground-state energy of the two-body problem under consideration.

For an attractive coupling constant $g < 0$ we find in the continuum limit ($L \to \infty$)

$$E = -\frac{g}{4}\,, \tag{C.21}$$

which is the only bound-state of the system in the continuum limit.

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Erklärung zur Dissertation

Hiermit versichere ich, die vorliegende Dissertation ohne Hilfe Dritter nur mit den angegebenen Quellen und Hilfsmitteln angefertigt zu haben. Alle Stellen, die aus Quellen entnommen wurden, sind als solche kenntlich gemacht. Diese Arbeit hat in gleicher oder ähnlicher Form noch keiner Prüfungsbehörde vorgelegen. Eine Promotion wurde bisher noch nicht versucht.

Darmstadt, den 22. Februar 2017

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